

Microwave Spectral Tables. III. Hydrocarbons, CH to C₁₀H₁₀

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Microwave Spectral Tables. III. Hydrocarbons, CH to C₁₀H₁₀

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All of the rotational spectral lines observed and reported in the open literature for 91 hydrocarbon molecules have been tabulated. This isotopic molecular species, assigned quantum numbers, observed frequency, estimated measurement uncertainty and reference are given for each transition reported. In addition to correcting a number of misprints and errors in the literature cited, the spectral lines for many normal isotopic species have been refit to produce a comprehensive and consistent analysis of all the data extracted from various literature sources. The derived molecular properties, such as rotational and centrifugal distortion constants, hyperfine structure constants, electric dipole moments, and rotational *g*-factors are listed.

Key words: dipole moments; hydrocarbons; hyperfine structure; internuclear distance; microwave spectra; rotational constants; rotational spectral lines.

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1. Introduction

These tables represent the third part of a series of critical reviews on molecular rotational spectra in the microwave frequency region. The present review on hydrocarbon species is a partial revision of the previous tabulation on polyatomic species, NBS Monograph 70, Vol. IV (1968)¹. The primary aim of the present critical review is directed at detecting errors, misprints and incomplete analyses in the literature. The coverage includes microwave rotational spectra and molecular properties derived therefrom for all the hydrocarbon species observed in the centimeter and millimeter wavelength region of the spectrum. There are two objectives which this review hopes to achieve: first, to provide an up-to-date and complete tabulation of the microwave spectra for hydrocarbon molecules, and second, to provide the best set of molecular properties which can be derived from the observed spectra. Although the spectral line frequencies are limited to the radio and microwave frequency region, derived molecular constants are included from a variety of sources, e.g., molecular beam electric resonance, electron paramagnetic resonance and infrared spectroscopy, in order to provide the most complete set of properties presently available. All unpublished data communicated privately have been included, and the open literature has been searched through September 1987.

1.1. General Description of the Tables

Two types of tables are presented for each molecular species. The first tables contain the derived molecular constants for each isotopic form which has been studied, and the table following these constant tables contains the observed microwave spectral transition frequencies for all isotopic forms and vibrational states for which data are available. The ordering of the tables follows an alphabetic sequence in empirical molecular formulas. The sequence of the tables is indicated in the List of Tables shown in the Contents.

The molecular spectral data tables of Sec. 2 are followed in Sec. 3 with the references to these data. Literature references are labeled with 5-digit numerals. This system has been formulated such that the first two digits refer to the year of publication of the work while the remaining three digits correspond to a chronological ordering within the year as required for referencing purposes here. Since this system was introduced in the earlier parts of this series^{2,3} these reference numbers follow the sequence established in the earlier work.

1.1.a. Molecular Constant Tables

Since a uniform format could not be readily constructed for these tables, they were composed in variable format depending on the type and amount of information available. In general, the rotational constants are listed first, followed by the centrifugal distortion parameters, hyperfine structure data, electric dipole moments and ro-

tational g-factors. In cases where extensive data are available, several individual tables are used to present the molecular constants. A more detailed description of the molecular constants and their symbols is given in Sec. 1.2. In order to reduce the occurrence of misprints, these tables were photographically reproduced from the original final typewritten copy.

1.1.b. Spectral Line Tables

The spectral tables contain all of the data intrinsic to an assigned molecular transition. The first column of these tables contains the isotopic molecular species to which the data pertain. The next columns contain the observed transition frequency and its estimated uncertainty. The next columns contain the assigned quantum numbers for the transition in the sequence: rotational and the hyperfine for the upper state, rotational and hyperfine for the lower state, and vibrational state designation. The reference to the original source of the data is given in the last column. Since the maximum number of significant figures beyond the decimal point was fixed at three for the transition frequency and uncertainties, in a few cases it was necessary to round off the measured data. This situation occurs primarily in the reproduction of molecular beam measurements. When uncertainties were not given in the original source, an uncertainty was assigned on the basis of the internal consistency of all the data available for the molecule in question. An effort was made to locate all of the essential references through mid-1987.

1.2. Molecular Parameters and Energy Level Formulation

The discussion which follows deals with the most common cases which will provide the user with the essential definition of quantum numbers, molecular parameters and basic relations employed in the analysis of rotational spectra. For the reader interested in a more detailed description of polyatomic rotational spectral measurements and analysis, we refer to texts on this subject by Townes and Schawlow⁴, Gordy and Cook⁵, Wollrab⁶ and Kroto⁷ which have both detailed and excellent discussions of all facets of rotational spectra. The spectroscopic notation employed follows, as closely as possible, the recommendations of the Joint Commission for Spectroscopy of the International Astronomic Union and the International Union of Pure and Applied Physics⁸.

1.2.a. Linear and Symmetric Top Molecules

The principal axes of a linear rigid rotor are along the molecular bond or *a*-axis for which the inertial moment is zero, and perpendicular to the bond axis in two orthogonal planes through the center-of-mass of the molecule. These are called the *b*- and *c*-axis whereby $I_c > I_b > I_a$ determines the labeling of the principal axes.

For linear molecules $I_b = I_c$ and $I_a = 0$, and the rotational constant, B , is related to the moment of the inertia as

$$B = \frac{h^2}{8\pi^2 I_b}$$

The selection rules for rotational transitions of a linear polyatomic molecule are $\Delta J = 0, \pm 1$, and $\Delta \ell = 0, \pm 1$ where J is the total angular momentum quantum number excluding nuclear spin and ℓ is the vibrational angular momentum quantum number which arises in degenerate bending vibrational states.

Since molecules are not rigid, the effects of molecular vibrations and centrifugal distortion must be included in the model in order to accurately fit the observed rotational spectra. The rotational energy levels are represented as:

$$F(J) = B_v[J(J+1) - \ell^2] - D_v[J(J+1) - \ell^2]^2 + H_v[J(J+1) - \ell^2]^3,$$

where B_v is the rotational constant for the n th vibrational state, and D_v and H_v are the centrifugal distortion constants. The rotational constant can be expressed in terms of its equilibrium value, B_e , and rotation-vibration interaction constants, α_j , as

$$B_v = B_{v_1, v_2, v_3} = B_e - \sum_{i=1,2,3} \alpha_i \left(v_i + \frac{d_i}{2} \right)$$

neglecting higher order terms. Within this level of approximation the frequencies of rotational transitions from lower state J'' to upper state $J' = J'' + 1$ are expressed:

$$\nu_{J \rightarrow J'} = 2B_v J' - 4D_v [(J')^3 - J' \ell^2] + 6J' H_v [(J')^4 + \frac{1}{3} J'^2 - 2(J')^2 \ell^2 + \ell^4].$$

The treatment of rotational transitions in excited vibrational states requires additional terms to account for the rotation-vibrational interactions. The symmetry species of excited vibrational states are designed as Σ, Π, Δ , etc., when $\ell = 0, \pm 1, \pm 2$, etc., respectively. One of the most common rotation-vibration interactions is ℓ -type doubling in Π states. In this case each $J \rightarrow J + 1$ transition has two components which are indicated as L (lower) and U (upper) components in the tables which follow. The doublet separation is represented as: $q_v(v+1)(J+1)$. In addition $\Delta J = 0$ transitions are observable with the frequency expressed as: $\nu = (q_v/2)(v+1)J(J+1)$. These transitions are also included in the spectral tables. Other rotation-vibration interactions, such as Fermi resonance, often must be included for particular measurements. Since the level of approximation and method of analysis is dependent on the extent and quality of the spectral measurements available, the user should refer to the literature references cited in the tables for details concerning the analysis. For more general treatments of ℓ -type doubling and resonance interactions see the texts mentioned earlier⁴⁻⁷ or the review by D.R. Lide⁹.

1.2.b. Symmetric Top Molecules

Like linear molecules, in a symmetric top one of the

principal axes must be coincident with the molecular symmetry axis, which must also be the axis with non-zero dipole moment. In a prolate symmetric top ($I_a < I_b = I_c$), the a-axis lies along the symmetry and in an oblate symmetric top ($I_a = I_b < I_c$). The rotational energy levels for the ground vibrational state of a symmetric top are represented as

$$E_{J,K} = BJ(J+1) + (A-B)K^2 - D_J J^2(J+1)^2 - D_{JK} J(J+1)K^2 - D_K K^4$$

including the first order (P^4) centrifugal distortion terms. The selection rules are $\Delta J = 0, \pm 1$, $\Delta K = 0$. The frequency for a $J+1 \leftarrow J$ and $K \leftarrow K$ rotational transition is

$$\nu = 2B_v J' - 4D_J (J')^3 - 2D_{JK} J' K^2 + H_{JJJ} (J')^3 [(J'+1)^3 - (J'-1)^3] + 4H_{JK} (J')^3 K^2 + 2H_{KK} J' K^4$$

which includes the P^6 centrifugal distortion terms.

As in the case of linear molecules, vibrationally excited states can exhibit ℓ -type doubling which arises from the degenerate bending vibrational modes. Formulas for the rotational levels are given in the references cited in the molecular parameter tables here, e.g., propyne references, as well as in some of the text books referenced here⁵⁻⁷.

1.2.c. Asymmetric Top Molecules

The majority of polyatomic molecules fall in the asymmetric-top category. When the three principal moments of inertia of a molecule differ, the molecule is classified as an asymmetric top. The energy level formulation for a rigid asymmetric top is considerably more complex than that for symmetric-tops or linear molecules. With the exception of low rotational levels, the rotational energy and transitions cannot be conveniently expressed in simple algebraic terms. Since Refs. 4-7 provide excellent discussions of the usual methods employed in solving the basic rigid asymmetric rotor Hamiltonian: $H_2 = A P_a^2 + B P_b^2 + C P_c^2$ as well as the more complex Hamiltonian which includes centrifugal distortion $H = H_2 + H_4 + H_6 + \dots$, we will not delve into any details of the quantum mechanical formulation, but concentrate on describing the quantum number designations employed in the tables to follow, and provide the basic relationships between the different molecular constant notations used by various authors.

The rotational energy levels are characterized by the three quantum numbers $J_{K_{-1}, K_{+1}}$ in the King-Hainer-Cross notation. Here, since $S = 0$, J is used rather than N for the rotational angular momentum. When $S \neq 0$ we will use $N_{K_{-1}, K_{+1}}$ to designate the rotational state and J for rotation plus electron spin and orbital angular momenta. The K_{-1} subscript is the K value in the limiting case of prolate symmetric-top and K_{+1} corresponds to the limiting case for an oblate symmetric-top. Ray's asymmetry parameter, κ , is often used to characterize the degree of asymmetry:

$$\kappa = \frac{2B - A - C}{A - C}$$

When $A \approx B$, κ approaches +1 for the oblate case and when $B \approx C$, κ approaches -1 for the prolate case.

(1) Selection Rules

In general an asymmetric rotor can exhibit three types of pure rotational transitions if the molecule has non-zero components of the electric dipole moment in the direction of the a , b , and c principal axes. For an asymmetric rotor the selection rules for a -type transitions are:

$$\Delta J = 0, \pm 1; \Delta K_{-1} = 0; \pm 2, \dots; \Delta K_{+1} = \pm 1, \mp 3, ,$$

for b -type transitions:

$$\Delta J = 0, \pm 1; \Delta K_{-1} = \pm 1, \pm 3, \Delta K_{+1} = \mp 1, \mp 3, \dots$$

for c -type transitions:

$$\Delta J = 0, \pm 1; \Delta K_{-1} = \pm 1, \pm 3; \Delta K_{+1} = 0, \mp 2.$$

When a molecule has a symmetry axis one must also examine the nuclear spin statistics which influence both the selection rules and the populations of the rotational levels.

(2) Rotational and Centrifugal Distortion Constants

Until approximately 1970 the Kivelson and Wilson¹⁰ formulation of the Hamiltonian for a non-rigid asymmetric rotor was widely employed in analyzing rotational spectra. With the parameter notation employed by Kirchhoff¹¹ the Kivelson-Wilson Hamiltonian is:

$$\mathcal{H} = A'P_a^2 + B'P_b^2 + C'P_c^2 + 1/4 \sum_{\alpha, \beta} \tau'_{\alpha\alpha\beta\beta} P_a^2 P_b^2, ,$$

where $\alpha, \beta = a, b$, or c . For a planar molecule the following planarity relations reduce the six linear combinations of distortion constants to four and provide the

determinable parameters shown in column 1 of Table 1.2.1:

$$\tau_{aac} = \tau_{bbc} = 0,$$

$$\tau_{aac} = \frac{C^2}{A^2} \tau_{aaa} + \frac{C^2}{B^2} \tau_{abb},$$

$$\tau_{bbc} = \frac{C^2}{B^2} \tau_{bbb} + \frac{C^2}{A^2} \tau_{abb},$$

$$\tau_{ccc} = \frac{C^2}{A^2} \tau_{aac} + \frac{C^2}{B^2} \tau_{bbc}.$$

For non-planar molecules Dreizler *et al.*^{12,13} found that the Kivelson-Wilson distortion constants were indeterminate. Watson^{14,15} introduced a new relationship which allows the Kivelson-Wilson Hamiltonian to be expressed in terms of five independent centrifugal distortion coefficients, or linear combinations of taus, which eliminates the indeterminacy noted by Dreizler *et al.* Much of the recent analysis of rotational spectra follows Watson's reformulation^{16,17} in the form of a reduced Hamiltonian which simplified the computation of the energy levels.

Since there is not a unique unitary transformation which allows the nine Kivelson-Wilson parameters to be reduced to eight determinable parameters, several variations of the Watson reduced Hamiltonian are commonly employed in practice. The two most often employed result in the determinable parameters listed in columns 2 and 3 of Table 1.2.1. In reanalyzing the microwave spectra here both Kirchhoff's¹¹ formulation has been used as well as Watson's A -reduction¹⁷. See reference¹¹ for additional details. The second commonly used formulation is described in detail by Gordy and Cook⁵. Yamada and Winnewisser¹⁸ have examined the effects of employing different reductions for the three King, Hainer and Cross axis representations I', II', and III'¹⁹. They provide a

TABLE 1.2.1. Determinable rotational and centrifugal distortion constants (P^4) employed by various workers^a

Kivelson-Wilson parameters for planar molecules	Kirchhoff parameters (following Watson ¹⁵)	Watson parameters ¹⁶
A'	$A'' = A' - 1/2\tau'_{bbc}$	\mathcal{A}
B'	$B'' = B' - 1/2\tau'_{aac}$	\mathcal{B}
C'	$C'' = C' - 1/2\tau'_{abb}$	\mathcal{C}
τ_{aaaa}	τ_{aaaa}	Δ_J
τ_{bbbb}	τ_{bbbb}	Δ_{JK}
τ_{abab}	τ_{cccc}	Δ_K
τ_{aabb}	$\tau_1 = \tau'_{aabb} + \tau'_{bbcc} + \tau'_{ccaa}$	δ_J
τ_{aabb}	$\tau_2 = (A'/S)\tau'_{bbcc} + (B'/S)\tau'_{aac} + (C'/S)\tau'_{aabb}$	δ_K
	$\tau_3 = [S/(B' - A')]\tau'_{aabb} + [S/(A' - C')]\tau'_{aac}$ + $[S/(C' - B')]\tau'_{bbcc}$	
	where $S = A' + B' + C'$	

^aFor conversion between the various sets of parameters see Refs. 4, 9, 10, and 17.

useful set of relations between the spectroscopic constants determined in the various reduction procedures and discuss the implications of the τ defect when employing the planarity conditions. When the spectral data require a higher order Hamiltonian, such as inclusion of P^6 terms, generally the first-order perturbation treatment suggested by Watson¹⁷ has been used.

1.2.d. Molecules with Doublet Electronic Ground States

The spectra and spectral analysis for molecules with one or more unpaired electrons are substantially more complex. The known hydrocarbon species that have doublet, $S=1/2$, ground states are HC_2 and HC_4 . In addition to the molecular rotational angular momentum, N , the interactions from electronic spin, S , and nuclear spin, I , must be included in the Hamiltonian. Depending on the magnitude of the various interactions, one of the following three coupling schemes are used in limiting cases:

- a) $N + S = J; J + I = F$
- b) $S + I = G; G + N = F$
- c) $N + I = E; E + S = F$

These interactions and the Hamiltonian for such molecules are discussed by Lin²⁰, Van Vleck²¹, Curl and Kinsey²² and others. Curl and Kinsey²² have summarized the spectroscopic constant notation employed in the various formulations and developed an alternate method which can be applied to the hydrocarbon species. Since none of these species have been reanalyzed in the present work, the notation employed in the publications cited is followed in the present tables of spectroscopic constants.

1.3. Evaluation of the Spectral Data

The evaluation has a two-fold purpose, first, the selection of the best set of measured transition frequencies and, second, selection or calculation of consistent and reliable spectroscopic constants. Since measured or calculated uncertainties are the best indicators of the quality of the data, a substantial portion of the critical evaluation effort has gone into determining these uncertainties.

1.3.a. General Procedure

Generally, the selection of the most reliable transition frequencies posed few problems since there were relatively few cases where duplicate measurements have been reported for the same transition and most laboratories quote reliable uncertainties. In cases where problems did occur, the selection was based on both the overall consistency of the measurement in question with the other spectral data available, and on the reported uncertainty in the measurements. In nearly all cases the measurements with the smallest uncertainties reported by the authors were found to be the most reliable.

The determination of the most reliable molecular constants posed more severe difficulties. Occasionally incon-

sistencies arose in cases where data were reported by several independent workers who studied quite different regions of the spectrum, e.g., molecular beam measurements vs microwave measurements or centimeter vs millimeter-wave measurements. If all of the available data had not been analyzed simultaneously in these instances, a reanalysis was carried out to eliminate the discrepancies. These calculations also resulted in the detection of a number of misprints in the literature which were not obvious through simple inspection of the reported assignments and transition frequencies. Since a question might arise concerning the correct value when a difference is noted between the present compilation and the reference cited, there are comments following the molecular constant tables in these cases.

1.4. List of Symbols

In most cases, a uniform set of quantum state and molecular parameter symbols is employed. This common set is listed here with a brief description of the molecular quantity represented by the symbol. However, there are a few special cases for which the reader is required to consult the literature cited to obtain this information since the Hamiltonian employed is unique to those species and reanalysis was not carried out here. The species for which the above applies are: CH , CH_2 , CH_4 , C_2H , CH_3CD_3 , C_3H , C_4H , and CH_3CCCD_3 . The spectra of these species were not refit in this work since the published analyses are considered to be accurate and not readily reproduced by the authors. There are several instances where excited vibrational states have been assigned and the type of vibrations identified, i.e. bend, torsion, etc., but the mode number is not identified. We have followed the notation in the literature and used the following characters for the type of vibration: B = bend, T = torsion, P = ring pucker.

1.4.a. Quantum Numbers

J	Resultant total angular momentum quantum number, excluding nuclear spins.
N	Rotational angular momentum quantum number, excluding electron and nuclear spins, in the case where electron spin is present.
K_-, K_+	Projection of J (or N) on the symmetry axis in the limiting prolate or oblate symmetric top.
F_1	Resultant angular momentum quantum number including nuclear spin for one nucleus.
F	Resultant total angular momentum quantum number.
A, E	Torsional symmetry substates representing irreducible representations of the symmetry group of the rotation-internal rotation Hamiltonian.
ν_1, ν_2, ν_3	Vibrational modes (ν) and quantum numbers (ν).

U or L Upper or lower energy level or transition frequency.
 ' or '' Prime or double prime is used to distinguish the upper (') and lower (') levels in a transition. They occur as superscripts on the quantum numbers.
 ℓ Quantum number for vibrational angular momentum.
 I (or I_i) Angular momentum quantum number of nuclear spin for one (or i th) nucleus.

1.4.c. Molecular Constants

A, B, C Rotational constants (MHz). These are related to the principal moments of inertia: $A = h/8\pi^2 I_a$, etc.
 B B -bar equals $(B + C)/2$.
 τ, Δ, δ, D Quartic centrifugal distortion constants (MHz or kHz).
 H, h Sextic centrifugal distortion constants (MHz or kHz).
 $L, \ell G, g$ Octic centrifugal distortion constants (MHz).
 I_a Moment of inertia of the methyl top around internal rotation axis ($\text{u } \text{\AA}^2$)
 ρ Internal rotation interaction constant $\rho = [\sum_x (\lambda_x I_a / I_x)^2]^{1/2}$.
 $\lambda_a, \lambda_b, \lambda_c$ Direction cosines between the internal rotation axis and the principal axes a, b, c respectively.
 α Angle of rotation around internal rotation axis.
 F Internal rotation dynamical constant (GHz) $F = h/8\pi^2 r I_a$.
 V_3 Threefold component of torsional barrier potential $V = V_3(1 - \cos 3\alpha)/2$.
 s Reduced barrier height $s = 4V_3/9F$.
 r $r = 1 - \sum_x (\lambda_x^2 I_a / I_x)$.
 Θ Angle between CH_3 symmetry axis and a -principal axis.
 $\omega_1(s)$ Fourier coefficient.
 Δ_0 Internal rotation interaction constant $\Delta_0 = 3Fa_1(s)/2 = \frac{28}{8}F \omega_1(s)$.
 μ_a, μ_b, μ_c Components of the electric dipole moment along the a - or b - or c -principal axes.
 α_v, γ_v Rotation-vibration coefficients in the power series representing B_v (see text).
 q_v ℓ -doubling constant (MHz).
 $\sigma_{\parallel}, \sigma_{\perp}$ Components of the magnetic shielding tensor which are parallel and perpendicular to the molecular axis, respectively.
 Q Molecular quadrupole moment relative to the center of mass ($\text{esu}\cdot\text{cm}^2$).
 $\alpha_{\parallel}, \alpha_{\perp}$ Electric polarizability anisotropy (cm^3).
 $\chi_{\perp}, \chi_{\parallel}$ Components of the magnetic susceptibility tensor which are respectively perpendicular and parallel to the molecular axis ($\text{erg/G}^2\cdot\text{mol}$).
 $\chi_{xx} - \chi_{yy}$ Magnetic susceptibility anisotropy.
 g_{\perp}, g_{\parallel} Components of the molecular G tensor which are respectively perpendicular and parallel to the molecular axis. g_{\perp} is sometimes denoted g or g_r for linear molecules in the ground state (μ_N).

$g_{xx} - g_{yy}$ Anisotropy of the molecular G tensor perpendicular to the molecular axis (μ_N).
 c_X or M Spin rotation constant related to nucleus X (kHz).
 S_{XY} Spin-spin interaction constant between nucleus X and nucleus Y (kHz).
 α_P, β_P Ω -type doubling parameters,

$$\alpha_P = 4\Sigma(-1)^s \times \frac{\langle \Pi | (A + 2B)L_y | \Sigma \rangle \langle \Sigma | BL_y | \Pi \rangle}{E_{\Sigma} - E_{\Pi}}$$

$$\beta_P = 4\Sigma(-1)^s \times \frac{|\langle \Pi | BL_y | \Sigma \rangle|^2}{E_{\Sigma} - E_{\Pi}}$$

p_{eff} Λ -type doubling constant in the $^2\Pi_{1/2}$ state (MHz).

a, b, c, d Magnetic hyperfine coupling constants (MHz) where,

$$a = 2\mu_B g_N \mu_N \langle 1/r^3 \rangle,$$

$$b = -\mu_B g_N \mu_N \left\langle \frac{3\cos^2\chi - 1}{r^3} \right\rangle + \frac{16}{3}\pi \mu_B g_N \mu_N \Psi^2(0),$$

$$c = 3\mu_B g_N \mu_N \left\langle \frac{3\cos^2\chi - 1}{r^3} \right\rangle,$$

$$d = 3\mu_B g_N \mu_N \left\langle \frac{\sin^2\chi - 1}{r^3} \right\rangle.$$

Here μ_B is the Bohr magneton, μ_N is the nuclear magneton and g_N is the nuclear g -value.
 A Spin-orbit coupling constants defined by the power series expansion, $A = A_c + A_{(1)} \xi + A_{(12)} \xi^2 + \dots$.

1.4.d. Other

X Refers to unknown uncertainty when appearing in the uncertainty column.

*

Asterisks in the uncertainty column indicate that the transition frequency is calculated rather than measured.

(...)

Parentheses in the numerical listings contain measured or estimated uncertainties. For example, the value 1.407(83) should be interpreted as 1.407 ± 0.083 . Thus the value in parentheses refers to the last significant digits given.

a, b, c Designate principal axes corresponding to A , B , and C , respectively.

1.5. Special Units, Fundamental Constants, and Useful Conversion Factors

1.5.a. Special Units

D Abbreviation for Debye units ($1 \text{ D} = 10^{-18}$ electrostatic units of charge \times centimeters, or $1 \text{ D} = 3.33564 \times 10^{-30}$ coulomb meter).

cm^{-1} Reciprocal wavelength (wave number) employed as a unit proportional to energy.
 \AA Angstrom abbreviation for the unit of length in bond distances ($1 \text{\AA} = 10^{-10} \text{ m}$).

1.5.b. Fundamental Constants and Conversion Factors²³

$A \cdot I_a = 5.0537905(85) \times 10^5 \text{ MHz} \cdot \text{u} \cdot \text{\AA}^2$,
 $h = 6.626176(36) \times 10^{-34} \text{ J} \cdot \text{s}$,
 $c = 2.99792458(1) \times 10^8 \text{ m} \cdot \text{s}^{-1}$
 $1 \text{ cm}^{-1} \cong 1.986478(11) \times 10^{-23} \text{ J}$,
 $\cong 11.96266 \text{ J mol}^{-1}$,
 $\cong 29979.2458 \text{ MHz}$,
 $1 \text{ u} = 1.6605655(86) \times 10^{-27} \text{ kg}$.

1.6. Acknowledgments

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2. Molecular Constants and Spectral Line Tables

As described in Sec. 1.1, the data tables for each molecule consist of a table of derived molecular constants followed by the spectral line table. These are ordered alphabetically by the empirical formula.

The molecular constants are presented for each isotopic species in the order: rotational constants, hyperfine structure constants, electric and magnetic dipole moments and, when appropriate, additional references which were not utilized in the tabulation. The molecular constants were either produced by our reanalysis of the data or then directly from the literature. A reference number in the table title means that all data is from that source. Reference numbers within the table refer only to the particular entry or column of entries. If no reference is given, the constants were determined in the present work. Reanalysis of the literature data focused on the normal isotopic species and ground vibrational states. For the most part the spectra for excited vibrational states and rare isotopic species were limited in quantum state covered. The published analyses, often rigid rotor fits, appeared accurate from inspection of the analyses.

The spectral line tables are organized first by isotopic species. For each species the transitions are listed by increasing frequency. All of the transitions listed after an isotopic species, formula belong to that species, since it is redundant to repeat these labels for every transition entry. The references to all data can be found in Sec. 3.

Table 1.1. Molecular constants for ^{12}CH and ^{13}CH .

Parameter	^{12}CH (MHz)	^{13}CH (MHz)
A_{O}	843817.57(69)	843806.97 ^a
B_{O}	425476.852(73)	422957.033 ^a
D_{O}	43.8255(32)	43.303 ^a
H_{O}	0.0035	0.00344 ^a
γ_{O}	-771.11(26)	-766.5 ^a
$\gamma_{D_{\text{O}}}$	0.158(24)	0.156 ^a
p	1003.9957(23)	998.44(25)
p_{D}	-0.27335(28)	-0.298(25)
p_{H}	-0.326(49) $\times 10^{-4}$	0.30 $\times 10^{-4}$ ^a
q	1159.6830(12)	1146.308(70)
q_{D}	-0.457479(47)	-0.4777(65)
q_{H}	0.9632(51) $\times 10^{-4}$	0.9404 $\times 10^{-4}$ ^a
$a(\text{H})$	54.28(14)	54.28 ^a
$b_{\text{F}}(\text{H})$	-57.67(20)	-57.67 ^a
$c(\text{H})$	57.17(17)	57.17 ^a
$d(\text{H})$	43.5167(40)	43.52 ^a
d_{D}	-0.01601(52)	---
C_{I}	0.0056(17)	0.504(101)
$a(^{13}\text{C})$		221.2(15)
$b_{\text{F}}(^{13}\text{C})$		46.8(20)
$c(^{13}\text{C})$		-127.8(23)
$d(^{13}\text{C})$		276.1(5)
Reference	[84033]	[86018]

^aCalculated from ^{12}CH parameters.

TABLE 1.2. Microwave spectrum of methylidyne radical

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' - J''$	$F' F_1' - F'' F_1''$	Vib. state	Ref.	
CH $^2\Pi_{1/2}$	3263.794	(0.003)	1/2 - 1/2	0 - 1	$\nu=0$	[74055]	
	3335.481	(0.002)	1/2 - 1/2	1 - 1	$\nu=0$	[74055]	
	3349.193	(0.003)	1/2 - 1/2	1 - 0	$\nu=0$	[74055]	
	7274.78	(0.15)	3/2 - 3/2	+1 - -2	$\nu=0$	[84033]	
	7325.15	(0.15)	3/2 - 3/2	+1 - -1	$\nu=0$	[84033]	
	7348.28	(0.15)	3/2 - 3/2	+2 - -2	$\nu=0$	[84033]	
	7398.38	(0.15)	3/2 - 3/2	+2 - -1	$\nu=0$	[84033]	
	14713.78	(0.15)	5/2 - 5/2	-2 - +3	$\nu=0$	[83012]	
	14756.81	(0.15)	5/2 - 5/2	-2 - +2	$\nu=0$	[83012]	
	14778.97	(0.20)	5/2 - 5/2	-3 - +3	$\nu=0$	[83012]	
	14821.88	(0.15)	5/2 - 5/2	-3 - +2	$\nu=0$	[83012]	
	24381.57	(0.40)	7/2 - 7/2	+3 - -4	$\nu=0$	[83012]	
	24420.65	(0.10)	7/2 - 7/2	+3 - -3	$\nu=0$	[83012]	
	24442.56	(0.10)	7/2 - 7/2	+4 - -4	$\nu=0$	[83012]	
	24482.10	(0.20)	7/2 - 7/2	+4 - -3	$\nu=0$	[83012]	
	50299.750	(0.020)	11/2 - 11/2	-5 - +5	$\nu=0$	[83028]	
	50321.276	(0.020)	11/2 - 11/2	-6 - +6	$\nu=0$	[83028]	
	66400.098	(0.030)	13/2 - 13/2	+6 - -6	$\nu=0$	[83028]	
	66421.466	(0.030)	13/2 - 13/2	+7 - -7	$\nu=0$	[83028]	
	CH $^2\Pi_{3/2}$	701.677	(0.010)	3/2 - 3/2	-2 - +2	$\nu=0$	[85016]
		724.789	(0.010)	3/2 - 3/2	-1 - +1	$\nu=0$	[85016]
		4847.84	(0.20)	5/2 - 5/2	+2 - -2	$\nu=0$	[83012]
		4870.12	(0.20)	5/2 - 5/2	+3 - -3	$\nu=0$	[83012]
11250.79		(0.50)	7/2 - 7/2	-4 - +3	$\nu=0$	[83012]	
11265.21		(0.15)	7/2 - 7/2	-4 - +4	$\nu=0$	[83012]	
11287.05		(0.15)	7/2 - 7/2	-3 - +3	$\nu=0$	[83012]	
11301.22		(0.20)	7/2 - 7/2	-3 - +4	$\nu=0$	[83012]	
43851.026		(0.030)	13/2 - 13/2	+7 - -7	$\nu=0$	[83028]	
43872.591		(0.030)	13/2 - 13/2	+6 - -6	$\nu=0$	[83028]	
58986.633		(0.020)	15/2 - 15/2	-8 - +8	$\nu=0$	[83028]	
59008.076		(0.020)	15/2 - 15/2	-7 - +7	$\nu=0$	[83028]	
76147.336		(0.030)	17/2 - 17/2	-9 - +9	$\nu=0$	[83028]	
76168.632		(0.050)	17/2 - 17/2	-8 - +8	$\nu=0$	[83028]	
$^{13}\text{C}\text{H } ^2\Pi_{1/2}$		3030.26	(1.00)	1/2 - 1/2	-0 1/2 - +1 3/2	$\nu=0$	[86018]
	3041.14	(1.25)	1/2 - 1/2	-0 1/2 - +1 1/2	$\nu=0$	[86018]	
	3323.30	(0.75)	1/2 - 1/2	-1 1/2 - +0 1/2	$\nu=0$	[86018]	
	3343.94	(1.30)	1/2 - 1/2	-1 1/2 - +1 3/2	$\nu=0$	[86018]	
	3355.73	(1.00)	1/2 - 1/2	-1 1/2 - +1 1/2	$\nu=0$	[86018]	
	3373.57	(0.75)	1/2 - 1/2	-1 3/2 - +0 1/2	$\nu=0$	[86018]	
	3394.58	(0.65)	1/2 - 1/2	-1 3/2 - +1 3/2	$\nu=0$	[86018]	
	3406.53	(2.00)	1/2 - 1/2	-1 3/2 - +1 1/2	$\nu=0$	[86018]	
	4712.13	(0.45)	5/2 - 5/2	+3 7/2 - -3 7/2	$\nu=0$	[86018]	
	4734.34	(0.60)	5/2 - 5/2	+3 5/2 - -3 5/2	$\nu=0$	[86018]	
	4743.92	(2.20)	5/2 - 5/2	+3 5/2 - -3 7/2	$\nu=0$	[86018]	
	4848.36	(2.50)	5/2 - 5/2	+2 5/2 - -2 3/2	$\nu=0$	[86018]	
	4855.63	(0.45)	5/2 - 5/2	+2 5/2 - -2 5/2	$\nu=0$	[86018]	
	4878.25	(0.60)	5/2 - 5/2	+2 3/2 - -2 3/2	$\nu=0$	[86018]	
	4887.73	(2.00)	5/2 - 5/2	+2 3/2 - -2 5/2	$\nu=0$	[86018]	
	4899.75	(1.80)	5/2 - 5/2	+3 7/2 - -2 5/2	$\nu=0$	[86018]	
	7093.95	(2.20)	3/2 - 3/2	+1 1/2 - -1 3/2	$\nu=0$	[86018]	
	7144.53	(1.50)	3/2 - 3/2	+1 1/2 - -1 1/2	$\nu=0$	[86018]	
	7159.27	(1.35)	3/2 - 3/2	+1 3/2 - -1 3/2	$\nu=0$	[86018]	
	7210.11	(1.20)	3/2 - 3/2	+1 3/2 - -1 1/2	$\nu=0$	[86018]	
	7245.41	(1.25)	3/2 - 3/2	+2 3/2 - -1 3/2	$\nu=0$	[86018]	
	7269.91	(1.30)	3/2 - 3/2	+2 3/2 - -2 3/2	$\nu=0$	[86018]	
	7309.94	(1.25)	3/2 - 3/2	+2 5/2 - -2 5/2	$\nu=0$	[86018]	
	7363.69	(2.00)	3/2 - 3/2	+2 5/2 - -2 3/2	$\nu=0$	[86018]	
	11047.51	(0.70)	7/2 - 7/2	-4 9/2 - +4 9/2	$\nu=0$	[86018]	
	11070.85	(1.00)	7/2 - 7/2	-4 7/2 - +4 7/2	$\nu=0$	[86018]	
	11190.16	(1.00)	7/2 - 7/2	-3 7/2 - +3 7/2	$\nu=0$	[86018]	
	11212.77	(1.20)	7/2 - 7/2	-3 5/2 - +3 5/2	$\nu=0$	[86018]	
	14458.28	(2.50)	5/2 - 5/2	-2 3/2 - +2 5/2	$\nu=0$	[86018]	
	14499.52	(0.80)	5/2 - 5/2	-2 3/2 - +2 3/2	$\nu=0$	[86018]	
14515.81	(0.70)	5/2 - 5/2	-2 5/2 - +2 5/2	$\nu=0$	[86018]		
14539.69	(2.50)	5/2 - 5/2	-2 3/2 - +3 5/2	$\nu=0$	[86018]		
14561.96	(2.00)	5/2 - 5/2	-3 5/2 - +2 5/2	$\nu=0$	[86018]		
14599.89	(2.20)	5/2 - 5/2	-2 5/2 - + 5/2	$\nu=0$	[86018]		

TABLE 1.2. Microwave spectrum of methylidyne radical — Continued

CH

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' - J''$	$F' F_1' - F'' F_1''$	Vib. state	Ref.
	14623.54	(2.20)	5/2 - 5/2	-3 7/2 - + 5/2	$\nu=0$	[86018]
	14643.93	(0.50)	5/2 - 5/2	-3 5/2 - + 5/2	$\nu=0$	[86018]
	14662.00	(0.50)	5/2 - 5/2	-3 7/2 - +3 7/2	$\nu=0$	[86018]
	14704.94	(2.50)	5/2 - 5/2	-3 7/2 - +3 5/2	$\nu=0$	[86018]

Table 2.1. Molecular parameters^a of CH₂(X³B₁).

Parameter	(000) State [82034]	(010) State [82033]
ν_O (cm ⁻¹)	---	963.09866(41)
A (cm ⁻¹)	73.05775(11)	184.12263(82)
B (cm ⁻¹)	8.415172(76)	8.36216(15)
C (cm ⁻¹)	7.219272(45)	7.09284(20)
Δ_K (cm ⁻¹)	1.991049(47)	23.969 ^b
Δ_{NK} (cm ⁻¹)	-0.019660(27)	-0.07889(14)
Δ_N (cm ⁻¹)	0.0003013(34)	0.000162(18)
δ_N (cm ⁻¹)	0.1012(12)x10 ⁻³	0.1012x10 ^{-3c}
ϕ_K (cm ⁻¹)	0.0	1.52 ^b
ϕ_{KN} (cm ⁻¹)	-0.0019417(21)	0.0
ϕ_{NK} (cm ⁻¹)	0.1281(186)x10 ⁻⁴	-4.671(57)x10 ⁻⁴
ϕ_N (cm ⁻¹)	0.251(59)x10 ⁻⁶	0.78(58)x10 ⁻⁶
ϕ'_N (cm ⁻¹)	0.195(30)x10 ⁻⁶	0.0
D (cm ⁻¹)	0.77842(14)	0.79560(48)
E (cm ⁻¹)	0.039906(38)	0.03540(53)
ϵ_{aa} (cm ⁻¹)	0.000446(78)	0.00352(54)
ϵ_{bb} (cm ⁻¹)	-0.005148(18)	-0.00470(23)
ϵ_{cc} (cm ⁻¹)	-0.004106(27)	-0.00458(21)
a_{FC} (MHz)	-20.26(51)	
T_{aa} (MHz)	39.7(17)	
T_{bb} (MHz)	-20.2(19)	

^aParameters not given were fixed at zero. The numbers in parentheses are one standard deviation from the least-squares fit in units of the last quoted digit.

^b Δ_K and ϕ_K were fixed at values determined from the semi-rigid bender model.

^c δ_N was fixed at its ground (000) state value.

Table 2.2. Molecular parameters^a for ¹³CH₂. [83049]

Parameter	(000) State	(010) State
ν_0 (cm ⁻¹)		959.1674(2)
A (cm ⁻¹)	72.627 ^b	181.23423(143)
B (cm ⁻¹)	8.415767(67)	8.37093(76)
C (cm ⁻¹)	7.208087(390)	7.07665(73)
Δ_K (cm ⁻¹)	2.583 ^b	23.657 ^b
Δ_{NK} (cm ⁻¹)	-0.01966 ^c	-0.07889 ^c
Δ_N (cm ⁻¹)	0.2569(156)x10 ⁻³	0.162x10 ^{-3c}
δ_N (cm ⁻¹)	0.1569(156)x10 ⁻³	0.3948(307)x10 ⁻³
ϕ_K (cm ⁻¹)	0.127 ^b	1.50 ^b
ϕ_{KN} (cm ⁻¹)	-0.19417x10 ^{-2c}	0
ϕ_{NK} (cm ⁻¹)	0.1281x10 ^{-4c}	-0.4671x10 ^{-3c}
ϕ_N (cm ⁻¹)	0.251x10 ^{-6c}	0.78x10 ^{-6c}
ϕ'_N (cm ⁻¹)	0.195x10 ^{-6c}	0
D (cm ⁻¹)	0.78006(130)	0.79767(37)
E (cm ⁻¹)	0.04176(53)	0.03839(137)
ϵ_{aa} (cm ⁻¹)	0.0446x10 ^{-2c}	0.352x10 ^{-2c}
ϵ_{bb} (cm ⁻¹)	-0.5148x10 ^{-2c}	-0.470x10 ^{-2c}
ϵ_{cc} (cm ⁻¹)	-0.4106x10 ^{-2c}	-0.458x10 ^{-2c}
a_{FC} (cm ⁻¹)	0.7955(185)x10 ⁻²	0.7330(209)x10 ⁻²
T_{aa} (cm ⁻¹)	-0.2173(748)x10 ⁻²	-0.2771(448)x10 ⁻²

^aParameters not given here were fixed at zero. The numbers in parentheses are on standard deviation from the least-squares fit in units of the last quoted digit.

^bThese parameters were fixed at values determined from a fit to nonrigid bender calculations for ¹³CH₂ by Jensen *et al.* [82032].

^cThese parameters were fixed to ¹²CH₂ values.

Table 2.3. Molecular parameters for the (000) and (010) vibrational levels of CD_2 in its X^3B_1 ground electronic state. [84028]

Parameter	(000) State ^a	(010) State ^b
ν_0	(cm^{-1})	752.3795(4)
A	(cm^{-1}) 37.786829(60)	70.45524(38)
$\frac{1}{2}(B+C)$	(cm^{-1}) 3.962159(12)	3.930017(27)
$\frac{1}{2}(B-C)$	(cm^{-1}) 0.26757(10)	0.3029(46)
Δ_K	(cm^{-1}) 0.560228(16)	4.991843(60)
Δ_{NK}	(cm^{-1}) $-0.49753(79) \times 10^{-2}$	$-0.019590(62)$
Δ_N	(cm^{-1}) $0.09242(63) \times 10^{-3}$	$0.1052(52) \times 10^{-3}$
δ_K	(cm^{-1}) $0.2783(50) \times 10^{-2}$	$1.71(23) \times 10^{-2}$
δ_N	(cm^{-1}) $0.2231(23) \times 10^{-4}$	$0.232(18) \times 10^{-4}$
ϕ_K	(cm^{-1}) 0.0196 ^c	0.278 ^c
ϕ_{KN}	(cm^{-1}) $-0.2433(19) \times 10^{-3}$	$-2.3749(66) \times 10^{-3}$
ϕ_{NK}	(cm^{-1}) $-0.189(18) \times 10^{-5}$	-0.189×10^{-5d}
ϕ_N	(cm^{-1}) 0 ^e	0 ^e
D	(cm^{-1}) 0.776466(93)	0.78935(24)
E	(cm^{-1}) 0.040580(65)	0.03727(24)
ϵ_{aa}	(cm^{-1}) $0.282(36) \times 10^{-3}$	$0.585(90) \times 10^{-3}$
$\frac{1}{2}(\epsilon_{bb} + \epsilon_{cc})$	(cm^{-1}) $-0.2342(19) \times 10^{-2}$	$-0.2420(48) \times 10^{-2}$
$\frac{1}{2}(\epsilon_{bb} - \epsilon_{cc})$	(cm^{-1}) $-0.262(18) \times 10^{-3}$	$-0.28(8) \times 10^{-3}$

^aFrom a fit to the previous far-infrared LMR data [83050] with the addition of the measurements of the $5_{23} + 5_{14}$ transition.

^bFrom a fit to ν_2 -band diode-laser measurements [83055] and the data of [84028]. For both states, magnetic g values were fixed at theoretical values, and the numbers in parentheses are one standard deviation from the least-squares fit expressed units of the last quoted digit.

^cFixed at a value determined from the energy levels given by Bunker and Jensen [83048].

^dFixed at the ground-state value.

^eThis parameter and all others not listed were fixed at zero.

TABLE 2.4. Microwave spectrum of methylene radical

CH₂

Isotopic species	Frequency (MHz)	Unc. (MHz)	N'(K ₋₁ ,K ₊₁) - N''(K ₋₁ ,K ₊₁)	J' F' ₁ - J'' F'' ₁	Vib. state	Ref.	
CH ₂ ³ B	68371.278	(0.041)	4(0, 4) - 3(1, 3)	5 6 - 4 5		[83046]	
	68375.875	(0.039)	4(0, 4) - 3(1, 3)	5 5 - 4 4		[83046]	
	68380.873	(0.041)	4(0, 4) - 3(1, 3)	5 4 - 4 3		[83046]	
	69007.179	(0.037)	4(0, 4) - 3(1, 3)	3 2 - 2 1		[83046]	
	69014.202	(0.037)	4(0, 4) - 3(1, 3)	3 3 - 2 2		[83046]	
	69019.187	(0.044)	4(0, 4) - 3(1, 3)	3 4 - 2 3		[83046]	
	69264.	(*10.)	4(0, 4) - 3(1, 3)			[82032]	
	70678.633	(0.042)	4(0, 4) - 3(1, 3)	4 3 - 3 2		[83046]	
	70679.543	(0.045)	4(0, 4) - 3(1, 3)	4 4 - 3 3		[83046]	
	70680.720	(0.038)	4(0, 4) - 3(1, 3)	4 5 - 3 4		[83046]	
	443314.	(*10.)	2(1, 2) - 3(0, 3)			[82032]	
	593016.	(*10.)	5(0, 5) - 4(1, 4)			[82032]	
	942752.	(*10.)	1(1, 1) - 2(0, 2)			[82032]	
	1797031.	(*10.)	1(1, 0) - 1(0, 1)			1ν ₁ [83048]	
	1835021.	(*10.)	2(1, 1) - 2(0, 2)			1ν ₁ [82032]	
	1892863.	(*10.)	3(1, 2) - 3(0, 3)			1ν ₁ [82032]	
	1915159.	(*10.)	1(1, 0) - 1(0, 1)			[82032]	
	1953602.	(*10.)	2(1, 1) - 2(0, 2)			[82032]	
	2012061.	(*10.)	3(1, 2) - 3(0, 3)			[82032]	
	2091456.	(*10.)	4(1, 3) - 4(0, 4)			[82032]	
	2317734.	(*10.)	6(1, 5) - 6(0, 6)			[82032]	
	2348016.	(*10.)	1(1, 1) - 0(0, 0)			[82032]	
	2650643.	(*10.)	2(1, 2) - 1(0, 1)			1ν ₁ [83048]	
	2782846.	(*10.)	2(1, 2) - 1(0, 1)			[82032]	
	2924276.	(*10.)	4(2, 2) - 5(1, 5)			[82032]	
	2930008.	(*10.)	3(2, 2) - 4(1, 3)			[82032]	
	4754102.	(*10.)	5(2, 3) - 5(1, 4)			[82032]	
	CD ₂ ³ B	515403.	(*10.)	1(1, 1) - 2(0, 2)			[83050]
		1005966.	(*10.)	1(1, 0) - 1(0, 1)			[83050]
		1022406.	(*10.)	2(1, 1) - 2(0, 2)			[83050]
		1047370.	(*10.)	3(1, 2) - 3(0, 3)			[83050]
		1227818.	(*10.)	1(1, 1) - 0(0, 0)			[83050]
		1450180.	(*10.)	2(1, 2) - 1(0, 1)			[83050]
1664966.		(*10.)	3(1, 3) - 2(0, 2)			[83050]	
1767106.		(*10.)	4(2, 2) - 5(1, 5)			[83050]	
1802739.		(*10.)	3(2, 2) - 4(1, 3)			[83050]	
2069063.		(*10.)	2(2, 1) - 3(1, 2)			[83050]	
2072840.		(*10.)	5(1, 5) - 4(0, 4)			[83050]	
2758720.		(*10.)	4(2, 2) - 4(1, 3)			[83050]	
2875172.		(*10.)	3(2, 1) - 3(1, 2)			[83050]	
2805872.		(*10.)	2(2, 0) - 2(1, 1)			[83050]	
2878376.		(*10.)	3(2, 2) - 3(1, 3)			[83050]	
2912514.		(*10.)	4(2, 3) - 4(1, 4)			[83050]	
3520937.		(*10.)	3(2, 2) - 2(1, 1)			[83050]	

Table 3.1. Molecular constants for CH₄ and ¹³CH₄.

Parameter	CH ₄	¹³ CH ₄
D _T (MHz)	0.13294357(97)	0.13298081(122)
H _{4T} (Hz)	-16.9790(90)	-16.9791(112)
H _{6T} (Hz)	10.9956(38)	11.1786(45)
L _{4T} (Hz)	2.000(23)x10 ⁻³	1.975(27)x10 ⁻³
L _{6T} (Hz)	-2.519(15)x10 ⁻³	-2.643(18)x10 ⁻³
L _{8T} (Hz)	-2.617(92)x10 ⁻³	-2.957(101)x10 ⁻³
Reference	[85020]	[86011]
<u>Distortion Dipole Moment</u> [71048], [78033]		
θ _Z ^{XY} (D) v ₁ =0	24.06(45)x10 ⁻⁶	
θ _Z ^{XY} (D) v ₁ =1	13.8(20)x10 ⁻⁶	
<u>Nuclear Hyperfine Constants</u> [80040]		
c _a (kHz)	10.372(83)	
c _d (kHz)	18.370(23)	
d (kHz)	21.17(32)	
Δ ₂ (kHz)	7970.30(66)	

Table 3.3. Molecular constants for CD₄ and ¹³CD₄.

Parameter	CD ₄	¹³ CD ₄
D _T (MHz)	0.03265087(89)	0.0326600(12)
H _{4T} (Hz)	-2.0281(40)	-2.0302(61)
H _{6T} (Hz)	1.1480(14)	1.1692(29)
L _{4T} (Hz)	0.1194(46)x10 ⁻³	0.1201(77)x10 ⁻³
L _{6T} (Hz)	-0.1431(28)x10 ⁻³	-0.1353(63)x10 ⁻³
L _{8T} (Hz)	-0.1560(85)x10 ⁻³	-0.1466(46)x10 ⁻³
Reference	[85020]	[87003]
<u>Distortion Dipole Moment</u> ¹³ CD ₄ [83054]		
θ _Z ^{XY} (D)	12.0(10)x10 ⁻⁶	

Table 3.2. Molecular constants for CH₃D and CH₂D₂.

Species	Parameter	Value	Reference
CH ₃ D	B _O (MHz)	116325.308(9)	[80039]
	μ _O J,K=1,1 (D)	5.641(3)x10 ⁻³	[70068]
	μ _O J,K=1,2 (D)	5.679(3)x10 ⁻³	[70068]
	eqQ(D) (kHz)	191.48(77)	[70068]
	c _α (kHz)	16.54(35)	[70068]
	c _β (kHz)	-1.58(100)	[70068]
CH ₂ D ₂	A-C (MHz)	37555.758	[75057]
	B-C (MHz)	13664.280	[75057]
	H _b (D)	0.014(5)	[75057]

TABLE 3.4. Microwave spectrum of methane

CH₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	<i>J'</i>	<i>C'</i>	<i>T'</i>	-	<i>J''</i>	<i>C''</i>	<i>T''</i>	Vib. state	Ref.	
CH ₄	7.970	(0.008)	2	<i>F</i> ₂	1	-	2	<i>E</i>	1		[81044]	
	423.02	(0.02)	7	<i>F</i> ₁	2	-	7	<i>F</i> ₂	2		[73082]	
	1246.55	(0.02)	7	<i>F</i> ₂	2	-	7	<i>F</i> ₁	1		[73082]	
	6895.204	(0.010)	6	<i>F</i> ₁	2	-	6	<i>F</i> ₂	2	1 <i>ν</i> ₃ <i>ℓ</i> = 7	[73083]	
	7861.703	(0.050)	14	<i>E</i>	3	-	14	<i>E</i>	2		[85020]	
	7944.957	(0.050)	12	<i>F</i> ₁	3	-	12	<i>F</i> ₂	1		[85020]	
	8570.956	(0.050)	16	<i>A</i> ₁	2	-	16	<i>A</i> ₂	1		[85020]	
	8620.452	(0.050)	16	<i>F</i> ₁	3	-	16	<i>F</i> ₂	2		[85020]	
	8652.563	(0.150)	15	<i>F</i> ₁	2	-	15	<i>F</i> ₂	2		[85020]	
	9046.922	(0.050)	14	<i>F</i> ₂	4	-	14	<i>F</i> ₁	2		[85020]	
	9361.072	(0.050)	11	<i>F</i> ₂	3	-	11	<i>F</i> ₁	1		[85020]	
	9591.270	(0.050)	19	<i>A</i> ₂	2	-	19	<i>A</i> ₁	1		[85020]	
	9894.238	(0.200)	16	<i>F</i> ₂	4	-	16	<i>F</i> ₁	3		[85020]	
	10321.942	(0.050)	12	<i>E</i>	2	-	12	<i>E</i>	1		[85020]	
	10373.540	(0.100)	16	<i>F</i> ₁	4	-	16	<i>F</i> ₂	3		[85020]	
	10474.550	(0.050)	14	<i>F</i> ₂	3	-	14	<i>F</i> ₁	1		[85020]	
	10519.185	(0.050)	13	<i>F</i> ₂	3	-	13	<i>F</i> ₁	2		[85020]	
	10652.609	(0.050)	17	<i>F</i> ₂	3	-	17	<i>F</i> ₁	3		[85020]	
	10797.985	(0.050)	12	<i>F</i> ₂	2	-	12	<i>F</i> ₁	1		[85020]	
	11261.362	(0.050)	13	<i>E</i>	2	-	13	<i>E</i>	1		[85020]	
	11421.276	(0.050)	15	<i>F</i> ₁	4	-	15	<i>F</i> ₂	3		[85020]	
	13154.727	(0.050)	17	<i>E</i>	3	-	17	<i>E</i>	2		[85020]	
	13279.651	(0.050)	12	<i>A</i> ₂	1	-	12	<i>A</i> ₁	1		[85020]	
	13401.780	(0.030)	9	<i>F</i> ₁	1	-	9	<i>F</i> ₁	1	1 <i>ν</i> ₄	[87013]	
	13663.922	(0.100)	15	<i>F</i> ₂	4	-	15	<i>F</i> ₁	2		[85020]	
	13675.008	(0.030)	5	<i>F</i> ₁	1	-	5	<i>F</i> ₁	1	1 <i>ν</i> ₄	[87013]	
	13845.458	(0.050)	13	<i>F</i> ₁	3	-	13	<i>F</i> ₂	1		[85020]	
	13915.890	(0.050)	17	<i>F</i> ₁	4	-	17	<i>F</i> ₂	2		[85020]	
	14030.436	(0.050)	12	<i>F</i> ₂	3	-	12	<i>F</i> ₁	1		[85020]	
	14151.879	(0.050)	15	<i>E</i>	2	-	15	<i>E</i>	1		[85020]	
	14776.843	(0.030)	2	<i>F</i> ₁	2	-	2	<i>F</i> ₁	2	1 <i>ν</i> ₄	[87013]	
	14850.910	(0.050)	13	<i>F</i> ₂	2	-	13	<i>F</i> ₁	1		[85020]	
	15146.857	(0.050)	15	<i>F</i> ₁	3	-	15	<i>F</i> ₂	2		[85020]	
	15401.529	(0.050)	14	<i>F</i> ₁	3	-	14	<i>F</i> ₂	2		[85020]	
	15601.846	(0.010)	6	<i>F</i> ₂	1	-	6	<i>F</i> ₁	2	1 <i>ν</i> ₃ <i>ℓ</i> = 7	[73083]	
	16289.143	(0.030)	3	<i>F</i> ₂	1	-	3	<i>F</i> ₂	2	1 <i>ν</i> ₄	[87013]	
	17821.123	(0.030)	5	<i>F</i> ₂	2	-	5	<i>F</i> ₂	2	1 <i>ν</i> ₄	[87013]	
	18106.641	(0.030)	5	<i>F</i> ₂	4	-	5	<i>F</i> ₂	3	1 <i>ν</i> ₄	[87013]	
	18528.94	(0.20)	18	<i>E</i>	3	-	18	<i>E</i>	2		[75056]	
	18562.40	(0.20)	16	<i>E</i>	3	-	16	<i>E</i>	2		[75056]	
	19288.63	(0.20)	13	<i>E</i>	2	-	13	<i>E</i>	1		[75056]	
	¹³ CH ₄	7865.140	(0.050)	14	<i>E</i>	2	-	14	<i>E</i>	1		[86011]
		7947.783	(0.050)	12	<i>F</i> ₁	3	-	12	<i>F</i> ₂	1		[86011]
		8571.452	(0.050)	16	<i>A</i> ₁	2	-	16	<i>A</i> ₂	1		[86011]
		8622.953	(0.050)	16	<i>F</i> ₁	3	-	16	<i>F</i> ₂	2		[86011]
		9051.096	(0.050)	14	<i>F</i> ₂	4	-	14	<i>F</i> ₁	2		[86011]
		9363.838	(0.050)	11	<i>F</i> ₂	3	-	11	<i>F</i> ₁	1		[86011]
9589.706		(0.050)	19	<i>A</i> ₂	2	-	19	<i>A</i> ₁	1		[86011]	
10324.129		(0.050)	12	<i>E</i>	2	-	12	<i>E</i>	1		[86011]	
10476.730		(0.050)	14	<i>F</i> ₂	3	-	14	<i>F</i> ₁	1		[86011]	
10523.128		(0.050)	13	<i>F</i> ₂	3	-	13	<i>F</i> ₁	2		[86011]	
10800.324		(0.050)	12	<i>F</i> ₂	2	-	12	<i>F</i> ₁	1		[86011]	
11265.530		(0.050)	13	<i>E</i>	2	-	13	<i>E</i>	1		[86011]	
11422.993		(0.030)	8	<i>F</i> ₂	1	-	8	<i>F</i> ₂	1	1 <i>ν</i> ₄	[87013]	
11426.496		(0.050)	15	<i>F</i> ₁	4	-	15	<i>F</i> ₂	3		[86011]	
12930.938		(0.030)	9	<i>F</i> ₁	1	-	9	<i>F</i> ₁	1	1 <i>ν</i> ₄	[87013]	
13111.090		(0.030)	5	<i>F</i> ₁	1	-	5	<i>F</i> ₁	1	1 <i>ν</i> ₄	[87013]	
13162.860		(0.050)	17	<i>E</i>	3	-	17	<i>E</i>	2		[86011]	
13283.732		(0.050)	12	<i>A</i> ₂	1	-	12	<i>A</i> ₁	1		[86011]	
13670.860		(0.050)	15	<i>F</i> ₂	4	-	15	<i>F</i> ₁	2		[86011]	
13848.256		(0.050)	13	<i>F</i> ₁	3	-	13	<i>F</i> ₂	1		[86011]	
13918.873		(0.050)	17	<i>F</i> ₁	4	-	17	<i>F</i> ₂	2		[86011]	
14085.537		(0.030)	2	<i>F</i> ₁	2	-	2	<i>F</i> ₁	2	1 <i>ν</i> ₄	[87013]	
14154.662		(0.050)	15	<i>E</i>	2	-	15	<i>E</i>	1		[86011]	
14854.204		(0.050)	13	<i>F</i> ₂	2	-	13	<i>F</i> ₁	1		[86011]	
15150.224	(0.050)	15	<i>F</i> ₁	3	-	15	<i>F</i> ₂	2		[86011]		
15407.437	(0.050)	14	<i>F</i> ₁	3	-	14	<i>F</i> ₂	2		[86011]		

TABLE 3.4. Microwave spectrum of methane — Continued

CH₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	<i>J'</i>	<i>C'</i>	<i>T'</i>	-	<i>J''</i>	<i>C''</i>	<i>T''</i>	Vib. state	Ref.
CD ₄	15559.539	(0.030)	3	F ₂	1	-	3	F ₂	2	1ν ₄	[87013]
	17117.264	(0.030)	5	F ₂	4	-	5	F ₂	3	1ν ₄	[87013]
	17260.660	(0.050)	14	A ₁	1	-	14	A ₂	1		[86011]
	17280.932	(0.030)	5	F ₂	2	-	5	F ₂	2	1ν ₄	[87013]
	17376.218	(0.050)	16	F ₁	4	-	16	F ₂	2		[86011]
	17965.454	(0.030)	6	F ₂	1	-	6	F ₂	1	1ν ₄	[87013]
	18532.82	(0.10)	18	E	3	-	18	E	2		[76059]
	18572.00	(0.12)	16	E	3	-	16	E	2		[76059]
	18585.000	(0.030)	6	F ₁	3	-	6	F ₁	3	1ν ₄	[87013]
	19292.80	(0.15)	14	E	2	-	14	E	1		[76059]
	104.236	(0.010)	7	F ₁	2	-	7	F ₂	2		[81045]
	125.033	(0.105)	21	F ₂	5	-	21	F ₁	6		[81045]
	385.310	(0.036)	7	F ₁	2	-	7	F ₂	1		[81045]
	1243.318	(0.046)	10	A ₁	1	-	10	A ₂	1		[85020]
	2452.846	(0.050)	19	A ₂	2	-	19	A ₁	1		[85020]
	8259.506	(0.050)	20	F ₁	4	-	20	F ₂	2		[85020]
	8266.767	(0.050)	18	F ₁	3	-	18	F ₂	2		[85020]
	8547.542	(0.050)	9	F ₂	1	-	9	F ₁	1	1ν ₄	[85021]
	8920.583	(0.050)	20	E	3	-	20	E	2		[85020]
	8998.854	(0.050)	19	E	2	-	19	E	1		[85020]
	9070.706	(0.050)	17	F ₂	2	-	17	F ₁	1		[85020]
	9266.154	(0.050)	5	F ₂	1	-	5	F ₁	1	1ν ₄	[85021]
	9324.892	(0.050)	19	F ₁	3	-	19	F ₂	2		[85020]
	9909.461	(0.050)	2	F ₂	2	-	2	F ₁	2	1ν ₄	[85021]
	10474.455	(0.050)	19	A ₁	1	-	19	A ₂	1		[85020]
	10548.114	(0.050)	18	A ₁	1	-	18	A ₂	1		[85020]
	10794.793	(0.050)	18	F ₁	2	-	18	F ₂	1		[85020]
	10851.117	(0.050)	19	F ₂	5	-	19	F ₁	2		[85020]
	10898.099	(0.050)	22	E	3	-	22	E	2		[85020]
	10990.119	(0.050)	3	F ₁	2	-	3	F ₂	1	1ν ₄	[85021]
	11011.867	(0.050)	20	F ₂	3	-	20	F ₁	2		[85020]
	11047.427	(0.050)	21	F ₂	4	-	21	F ₁	3		[85020]
	11493.446	(0.050)	22	F ₂	4	-	22	F ₁	2		[85020]
	11642.592	(0.050)	20	F ₁	3	-	20	F ₂	1		[85020]
	11915.304	(0.050)	23	E	3	-	23	E	2		[85020]
	12457.713	(0.050)	6	F ₁	1	-	6	F ₂	1	1ν ₄	[85021]
	12500.125	(0.050)	6	F ₂	3	-	6	F ₁	3	1ν ₄	[85021]
	12626.803	(0.050)	10	A ₂	1	-	10	A ₁	1	1ν ₄	[85021]
	12788.210	(0.050)	19	F ₁	2	-	19	F ₂	1		[85020]
	12896.520	(0.050)	5	F ₁	3	-	5	F ₂	4	1ν ₄	[85021]
	12921.335	(0.050)	21	A ₂	1	-	21	A ₁	1		[85020]
	13090.017	(0.050)	11	F ₁	7	-	11	F ₂	6	1ν ₄	[85021]
	13297.122	(0.050)	23	F ₁	4	-	23	F ₂	3		[85020]
	13523.924	(0.050)	21	F ₂	3	-	21	F ₁	2		[85020]
	14054.956	(0.050)	22	A ₂	2	-	22	A ₁	1		[85020]
14159.642	(0.050)	8	F ₂	5	-	8	F ₁	5	1ν ₄	[85021]	
14183.737	(0.050)	9	F ₁	4	-	9	F ₂	5	1ν ₄	[85021]	
14428.237	(0.050)	23	F ₂	4	-	23	F ₁	2		[85020]	
15157.079	(0.050)	24	A ₁	2	-	24	A ₂	1		[85020]	
15262.206	(0.050)	20	F ₂	2	-	20	F ₁	1		[85020]	
15414.963	(0.050)	12	F ₂	6	-	12	F ₁	6	1ν ₄	[85021]	
15675.150	(0.050)	22	F ₂	3	-	22	F ₁	1		[85020]	
¹³ CD ₄	698.843	(0.052)	22	F ₁	4	-	22	F ₂	5		[87003]
	911.938	(0.056)	12	F ₂	3	-	12	F ₂	2		[87003]
	923.452	(0.042)	12	F ₂	2	-	12	F ₁	2		[87003]
	1718.910	(0.051)	12	F ₂	3	-	12	F ₁	2		[87003]
	2106.762	(0.014)	21	F ₂	4	-	21	F ₁	4		[87003]
	3156.452	(0.077)	21	F ₁	4	-	21	F ₂	3		[87003]
	4416.682	(0.090)	22	F ₁	4	-	22	F ₂	4		[83054]
	8788.073	(0.077)	17	F ₁	3	-	17	F ₂	1		[87003]
	8788.285	(0.078)	21	F ₁	4	-	21	F ₂	2		[87003]
	9072.496	(0.045)	17	F ₂	2	-	17	F ₁	1		[87003]
	9144.378	(0.056)	21	F ₂	5	-	21	F ₁	4		[87003]
	9378.446	(0.007)	22	F ₁	4	-	22	F ₂	3		[87003]
	11369.124	(0.080)	5	F ₂	4	-	5	F ₁	3	1ν ₄	[87003]
	11453.252	(1.25)	17	F ₂	1	-	17	F ₁	1		[87003]

TABLE 3.4. Microwave spectrum of methane — Continued

CH₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	<i>J'</i>	<i>C'</i>	<i>T'</i>	-	<i>J''</i>	<i>C''</i>	<i>T''</i>	Vib. state	Ref.
CH ₃ D	232644.327	(0.018)		1(0, 0)		-	0(0, 0)				[80039]
CH ₂ D ₂	37556.666	(0.050)		1(1, 0)		-	1(0, 1)				[75057]
	55617.92	(0.05)		2(1, 1)		-	2(0, 2)				[75057]
	74188.234	(0.050)		3(2, 1)		-	3(1, 2)				[75057]

Table 4.1. Molecular constants for the ethynyl radical.

Parameter	CCR	CGD
B (MHz)	43674.542(8)	36068.035(14)
D (MHz)	0.1076(8)	0.0687(7)
γ (MHz)	-62.647(35)	-55.84(3)
b (MHz)	40.54(20)	6.35(7)
c (MHz)	12.26(26)	1.59(26)
eqQ (MHz)		0.21(9)
Reference	[83008]	[85007],[85000]

TABLE 4.2. Microwave spectrum of ethynyl radical

C₂H

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' - J''$	P	$F' - F''$	Vib. state	Ref.	
CCH	87284.156	(0.030)	3/2 - 1/2		1 - 1	$\nu = 0$	[83008]	
	87316.924	(0.010)	3/2 - 1/2		2 - 1	$\nu = 0$	[83008]	
	87328.623	(0.016)	3/2 - 1/2		1 - 0	$\nu = 0$	[83008]	
	87402.037	(0.040)	1/2 - 1/2		1 - 1	$\nu = 0$	[83008]	
	87407.165	(0.011)	1/2 - 1/2		1 - 0	$\nu = 0$	[83008]	
	87446.512	(0.023)	1/2 - 1/2		0 - 1	$\nu = 0$	[83008]	
	170885.841	(0.082)	3/2 - 1/2		-	1 - 0	$\nu = 1$	[87027]
	170887.030	(0.029)	3/2 - 1/2		-	2 - 1	$\nu = 1$	[87027]
	170897.890	(0.042)	3/2 - 1/2		-	1 - 1	$\nu = 1$	[87027]
	172246.787	(0.046)	3/2 - 1/2		+	1 - 0	$\nu = 1$	[87027]
	172249.761	(0.020)	3/2 - 1/2		+	2 - 1	$\nu = 1$	[87027]
	172263.532	(0.038)	3/2 - 1/2		+	1 - 1	$\nu = 1$	[87027]
	172263.532	(0.038)	3/2 - 1/2		+	1 - 1	$\nu = 1$	[87027]
	172263.532	(0.038)	3/2 - 1/2		+	1 - 1	$\nu = 1$	[87027]
	174215.440	(0.026)	5/2 - 3/2		-	3 - 2	$\nu = 1$	[87027]
	174219.435	(0.042)	5/2 - 3/2		-	2 - 1	$\nu = 1$	[87027]
	174663.222	(0.008)	5/2 - 3/2			3 - 2	$\nu = 0$	[83008]
	174667.685	(0.017)	5/2 - 3/2			2 - 1	$\nu = 0$	[83008]
	174721.777	(0.026)	3/2 - 1/2			2 - 1	$\nu = 0$	[83008]
	174728.100	(0.040)	3/2 - 1/2			1 - 1	$\nu = 0$	[83008]
	175575.067	(0.095)	5/2 - 3/2		+	3 - 2	$\nu = 1$	[87027]
	175578.769	(0.041)	5/2 - 3/2		+	2 - 1	$\nu = 1$	[87027]
	259152.150	(0.038)	5/2 - 3/2		+		$\nu = 1$	[87027]
	260447.247	(0.032)	7/2 - 5/2		+	4 - 3	$\nu = 1$	[87027]
	260448.876	(0.032)	7/2 - 5/2		+	3 - 2	$\nu = 1$	[87027]
	261196.725	(0.038)	5/2 - 3/2		-		$\nu = 1$	[87027]
	262004.260	(0.100)	7/2 - 5/2			4 - 3	$\nu = 0$	[81041]
	262006.482	(0.100)	7/2 - 5/2			3 - 2	$\nu = 0$	[81041]
	262064.986	(0.100)	5/2 - 3/2			3 - 2	$\nu = 0$	[81041]
	262067.469	(0.100)	5/2 - 3/2			2 - 1	$\nu = 0$	[81041]
	262487.823	(0.020)	7/2 - 5/2		-	4 - 3	$\nu = 1$	[87027]
	262489.430	(0.024)	7/2 - 5/2		-	3 - 2	$\nu = 1$	[87027]
	346249.035	(0.050)	7/2 - 5/2		-		$\nu = 1$	[87027]
	346928.993	(0.037)	9/2 - 5/2		-		$\nu = 1$	[87027]
	348974.523	(0.054)	7/2 - 5/2		+		$\nu = 1$	[87027]
	349338.103	(0.100)	9/2 - 7/2				$\nu = 0$	[81041]
349400.612	(0.100)	7/2 - 5/2				$\nu = 0$	[81041]	
CCD	72107.70	(0.03)	3/2 - 1/2		5/2 - 3/2	$\nu = 0$	[85000]	
	144241.91	(0.03)	5/2 - 3/2		7/2 - 5/2	$\nu = 0$	[85000]	
	144243.06	(0.03)	5/2 - 3/2		5/2 - 3/2	$\nu = 0$	[85000]	
	144243.06	(0.03)	5/2 - 3/2		3/2 - 1/2	$\nu = 0$	[85000]	
	144237.11	(0.03)	5/2 - 3/2		5/2 - 5/2	$\nu = 0$	[85000]	
	144239.71	(0.03)	5/2 - 3/2		3/2 - 3/2	$\nu = 0$	[85000]	
	144296.72	(0.03)	3/2 - 1/2		5/2 - 3/2	$\nu = 0$	[85000]	
	144297.66	(0.03)	3/2 - 1/2		3/2 - 1/2	$\nu = 0$	[85000]	
	144299.21	(0.03)	3/2 - 1/2		3/2 - 3/2	$\nu = 0$	[85000]	
	144299.21	(0.03)	3/2 - 1/2		1/2 - 1/2	$\nu = 0$	[85000]	
	216368.56	(0.05)	7/2 - 5/2		7/2 - 7/2	$\nu = 0$	[85007]	
	216369.99	(0.07)	7/2 - 5/2		5/2 - 5/2	$\nu = 0$	[85007]	
	216372.83	(0.02)	7/2 - 5/2		9/2 - 7/2	$\nu = 0$	[85007]	
	216373.32	(0.02)	7/2 - 5/2		7/2 - 5/2	$\nu = 0$	[85007]	
	216373.32	(0.02)	7/2 - 5/2		5/2 - 3/2	$\nu = 0$	[85007]	
	216428.32	(0.02)	5/2 - 3/2		7/2 - 5/2	$\nu = 0$	[85007]	
	216428.32	(0.02)	5/2 - 3/2		5/2 - 3/2	$\nu = 0$	[85007]	
	216428.76	(0.04)	5/2 - 3/2		3/2 - 1/2	$\nu = 0$	[85007]	
	216430.34	(0.06)	5/2 - 3/2		3/2 - 3/2	$\nu = 0$	[85007]	
	216431.26	(0.05)	5/2 - 3/2		5/2 - 5/2	$\nu = 0$	[85007]	
	288499.00	(0.05)	9/2 - 7/2				$\nu = 0$	[85000]
	288554.59	(0.05)	7/2 - 5/2				$\nu = 0$	[85000]
	360618.34	(0.15)	11/2 - 9/2				$\nu = 0$	[85000]
	360674.17	(0.15)	9/2 - 7/2				$\nu = 0$	[85000]

Table 5.1. Molecular constants for d_1 -acetylene (HCCD).

Parameter	Ground State	ν_4	ν_5
B_0 (MHz)	29725.24(5)	29803.003(6)	29766.750(4)
D_0 (MHz)	0.0336(32)		
D_c (MHz)		0.0363(9)	0.0342(2)
D_d (MHz)		0.0303(12)	0.0352(3)
q_v (MHz)		132.993(14)	105.702(8)
μ_v (D)		0.02359(5)	0.05601(9)
Reference	[69062]	[80037]	[80037]
		<u>$3\nu_4(\Pi)$</u>	<u>$3\nu_5(\Pi)$</u>
B_v (MHz)		29969.052(43)	29861.189(27)
D_c (MHz)			0.0402(9)
D_d (MHz)			0.0450(12)
q_v (MHz)		135.529(25)	108.642(28)
μ_v (D)		0.090077(26)	0.1472(21)
Reference		[80037]	[80037]

Table 5.2. Molecular constants for DCCD from the $\nu_5^1 - \nu_4^1$ band. [77038]

Parameter	Value
ν_0 (cm^{-1})	27.10461(19)
B_4 (MHz)	25480.70(43)
B_5 (MHz)	25483.24(46)
D_4 (MHz)	0.02436(19)
D_5 (MHz)	0.02427(23)
q_4 (MHz)	97.02(18)
q_5 (MHz)	98.02(22)
ν_4 (MHz)	0.00023(17)
ν_5 (MHz)	0.00013(21)
$B_5 - B_4$ (MHz)	2.537(34)
$q_5 - q_4$ (MHz)	0.992(16)
$D_5 - D_4$ (MHz)	-0.000083(49)
Deuterium hyperfine constants [87023]	
eQq (ν_4) (MHz)	0.20916
eQq (ν_5) (MHz)	0.20870
c (ν_4) (MHz)	-0.44×10^{-4}
c (ν_5) (MHz)	$-0.40 \times 10^{-\sigma}$

TABLE 5.3. Microwave spectrum of acetylene

C₂H₂

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' - J''$	Vib. state	Ref.	
HCCD	59450.6	(0.2)	1 - 0		[64029]	
	118854.778	(0.019)	2 - 1	1 ν_5 c	[80037]	
	118945.132	(0.017)	2 - 1	1 ν_4 c	[80037]	
	119009.24	(0.15)	2 - 1	3 ν_5 c	[80037]	
	119277.553	(0.019)	2 - 1	1 ν_5 d	[80037]	
	119333.134	(0.039)	2 - 1	3 ν_4 c	[80037]	
	119477.295	(0.017)	2 - 1	1 ν_4 d	[80037]	
	119878.22	(0.15)	2 - 1	3 ν_5 d	[80037]	
	120417.362	(0.039)	2 - 1	3 ν_4 d	[80037]	
	DCCD	47672.55	(0.05)	14 - 15	1 ν_4 - 1 ν_5 d	[77038]
		50367.48	(0.05)	14 - 15	1 ν_4 - 1 ν_5 c	[77038]
51084.63		(0.05)	17 - 16	1 ν_5 - 1 ν_4 c	[77038]	
54101.63		(0.05)	17 - 16	1 ν_5 - 1 ν_4 d	[77038]	
98582.83		(0.05)	13 - 14	1 ν_4 - 1 ν_5 d	[77038]	
101789.73		(0.05)	18 - 17	1 ν_5 - 1 ν_4 c	[77038]	
101113.20		(0.15)	13 - 14	1 ν_4 - 1 ν_5 c	[77038]	
104964.42		(0.05)	18 - 17	1 ν_5 - 1 ν_4 d	[77038]	

Table 6.1. Molecular constants for deuterated ethylene [81042].

Parameter	CH ₂ CD ₂ (MHz)	CH ₂ CHD (MHz)	cis-CHDCHD (MHz)
A	97496.7(18) ^a	120093.521(70) ^a	99667.262(89)
B	25675.260(44)	27470.737(26)	25417.208(41)
C	20268.791(40)	22297.745(14)	20199.073(24)
Δ_K	(1.224) ^b	2.1164(34)	1.4589(63)
Δ_{JK}	0.1919(28)	0.1804(45)	0.117(11)
Δ_J	0.03273(5)	0.03903(53)	0.0359(12)
δ_J	0.00788(13)	0.008405(63)	0.008648(98)
δ_K	0.206(22)	0.2438(43)	0.1966(66)
μ (D)	0.0091(4)		

^aUncertainties in parentheses are 2.5 standard deviations.^bValue from J.L. Duncan, D.C. McKear, and P.S. Mallinson, J. Mol. Spectrosc. 45, 221 (1973).

TABLE 6.2. Microwave spectrum of ethylene

C₂H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
CH ₂ CHD	99325.280	(0.050)	2(0, 2) - 1(0, 1)	[81042]
	103174.346	(0.050)	2(1, 1) - 2(0, 2)	[81042]
	104706.688	(0.050)	2(1, 1) - 1(1, 0)	[81042]
	111635.872	(0.050)	3(1, 2) - 3(0, 3)	[81042]
	116368.314	(0.050)	4(0, 4) - 3(1, 3)	[81042]
	123623.433	(0.050)	4(1, 3) - 4(0, 4)	[81042]
	130218.210	(0.050)	7(1, 6) - 6(2, 5)	[81042]
	133418.797	(0.050)	6(3, 3) - 7(2, 6)	[81042]
	139677.511	(0.050)	5(1, 4) - 5(0, 5)	[81042]
	141414.091	(0.050)	3(1, 3) - 2(1, 2)	[81042]
	142389.091	(0.050)	1(1, 1) - 0(0, 0)	[81042]
	142405.002	(0.050)	13(5, 9) - 14(4, 10)	[81042]
	147157.056	(0.050)	13(5, 8) - 14(4, 11)	[81042]
	149296.905	(0.050)	3(2, 2) - 2(2, 1)	[81042]
	150136.632	(0.050)	3(2, 1) - 2(2, 0)	[81042]
	154766.524	(0.050)	9(4, 6) - 10(3, 7)	[81042]
	156573.485	(0.050)	11(2, 9) - 10(3, 8)	[81042]
	156923.058	(0.050)	3(1, 2) - 2(1, 1)	[81042]
	159588.607	(0.050)	15(3, 12) - 14(4, 11)	[81042]
	CH ₂ CD ₂	160356.907	(0.050)	6(1, 5) - 6(0, 6)
163685.633		(0.050)	9(4, 5) - 10(3, 8)	[81042]
45943.928		(0.050)	1(0, 1) - 0(0, 0)	[81042]
53090.598		(0.050)	8(2, 6) - 8(2, 7)	[81042]
62937.912		(0.050)	13(3, 10) - 13(3, 11)	[81042]
78305.078		(0.050)	9(2, 7) - 9(2, 8)	[81042]
86480.818		(0.050)	2(1, 2) - 1(1, 1)	[81042]
89944.923		(0.050)	14(3, 11) - 14(3, 12)	[81042]
91593.381		(0.050)	2(0, 2) - 1(0, 1)	[81042]
109211.211		(0.050)	10(2, 8) - 10(2, 9)	[81042]
123173.558		(0.050)	15(3, 12) - 15(3, 13)	[81042]
129541.200		(0.050)	3(1, 3) - 2(1, 2)	[81042]
136659.623		(0.050)	3(0, 3) - 2(0, 2)	[81042]
137824.016		(0.050)	3(2, 2) - 2(2, 1)	[81042]
138993.053		(0.050)	3(2, 1) - 2(2, 0)	[81042]
145746.403		(0.050)	3(1, 2) - 2(1, 1)	[81042]
172399.023		(0.050)	4(1, 4) - 3(1, 3)	[81042]
180882.216		(0.050)	4(0, 4) - 3(0, 3)	[81042]
183533.569		(0.050)	4(2, 3) - 3(2, 2)	[81042]
c-CHDCHD		66491.771	(0.050)	3(0, 3) - 2(1, 2)
	79466.095	(0.050)	1(1, 0) - 1(0, 1)	[81042]
	84947.955	(0.050)	2(1, 1) - 2(0, 2)	[81042]
	93658.879	(0.050)	3(1, 2) - 3(0, 3)	[81042]
	94342.540	(0.050)	6(1, 5) - 5(2, 4)	[81042]
	106146.344	(0.050)	4(1, 3) - 4(0, 4)	[81042]
	115339.012	(0.050)	8(4, 5) - 9(3, 6)	[81042]
	117477.979	(0.050)	4(0, 4) - 3(1, 3)	[81042]
	119864.960	(0.050)	1(1, 1) - 0(0, 0)	[81042]
	122880.431	(0.050)	8(4, 4) - 9(3, 7)	[81042]
	123042.478	(0.050)	5(1, 4) - 5(0, 5)	[81042]
	144932.159	(0.050)	6(1, 5) - 6(0, 6)	[81042]
	155362.920	(0.050)	7(1, 6) - 6(2, 5)	[81042]
	160262.662	(0.050)	2(1, 2) - 1(0, 1)	[81042]
	172182.699	(0.050)	7(1, 6) - 7(0, 7)	[81042]

Table 7.1. Molecular constants for ^{12}C and ^{13}C isotopic forms of CH_3CD_3 .

Parameter	CH_3CD_3	$^{13}\text{CH}_3\text{CD}_3$	$\text{CH}_3^{13}\text{CD}_3$
B (MHz)	16503.81(81)	16088.428(30)	16251.914(30)
D_J (MHz)	0.0195(14)		
D_{JK} (MHz)	0.0493(66)		
D_K (MHz)	0.1421		
ρ	0.3339792(22)		
V_3 (cm^{-1})	1004.13(21)		
F (MHz)	-143.(9)		
D_{Jm} (MHz)	2.55(9)		
d_J (MHz)	6.18(27)		
I_α ($\text{u } \text{Å}^2$)	3.1549(12) ^a		
μ_0 (D)	0.0108617(5)	0.01067(10)	0.01096(11)
μ_1 (D)	0.01107(11) ^b		
$(\alpha_{\parallel} - \alpha_{\perp})$ (10^{-24}cm^3)	0.672(27)		
g_{\parallel} (μ_N)	+0.16451(25)		
g_{\perp} (μ_N)	+0.00325(16)		
$(\chi_{\parallel} - \chi_{\perp})$ (10^{-3}J/T^2)	-90.2(15)		
Reference	[84030]	[77039]	[77039]

^aCalculated from $\rho = I_\alpha / (I_\alpha + I_F)$ using $I_a = 9.4965(20) \text{ u } \text{Å}^2$.

^bReference [71047].

Table 7.2. Molecular constants for CH_3CHD_2 .

Parameter	Ground State [79037]	Torsionally Excited State ^b [81043]
A (MHz)	60809.592(5)	60847.(106)
B (MHz)	17770.87(16)	17703.167(48)
C (MHz)	17084.84(16)	17030.976(54)
Δ_J (MHz)	0.02333(45)	
Δ_{JK} (MHz)	0.0602(20)	
Δ_K (MHz)	0.177(15)	
δ_J (MHz)	0.00079(16)	
δ_K (MHz)	0.050(81)	
D (MHz)	-566.319 \pm 50 ^a	
F (GHz)	257.70(35)	
V_3 (cm^{-1})	1007.4(9)	1003.0(6)

^aAssumed value.

^bCentrifugal distortion, F and D values assumed to be the same as the ground state.

Table 7.3. Molecular constants of CH₃CH₂D, CD₃CH₂D and gauche-CH₂DCH₂D. [81043]

Parameter	CH ₃ CH ₂ D	CD ₃ CH ₂ D	g-CH ₂ DCH ₂ D
A (MHz)	69640.504(69) ^a	48650.630(58)	61360.344(23)
B (MHz)	18876.23(14)	15656.793(64)	17642.0291(75)
C (MHz)	18209.90(13)	15194.324(63)	17036.3299(75)
Δ _J (MHz)	0.02661(52)	0.01752(14)	0.024596(66)
Δ _{JK} (MHz)	0.0673(13)	0.04093(57)	0.04976(10)
Δ _K (MHz)	0.243(16)	0.100(15)	0.1963(35)
δ _J (MHz)	0.00103(17)	0.000576(65)	0.00107276(91)
δ _K (MHz)	-0.057(65)	-0.050(30)	0.18252(48)
D (MHz)	(811.64) ^b	(611.36) ^b	
F (GHz)	282.795(49)	203.49(65)	
V ₃ (cm ⁻¹)	1010.90(12)	651.7(38)	

^aValues in parentheses denote 2.5 standard errors and apply to the last digits of constants.

^bFixed. These values were obtained in the same way as in the case of CH₃CHD₂ (see Ref.(1)).

^cFixed.

TABLE 7.4. Microwave spectrum of ethane

C₂H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$	$- J''(K_{-1}, K_{+1})$	ν_1	Sym.	Vib. state	Ref.
CH ₃ CD ₃	65896.92	(0.05)	2(1, 0)	- 1(1, 0)				[71047]
	65675.54	(0.05)	2(1, 0)	- 1(1, 0)			1v ₆	[71047]
	98843.31	(0.15)	3(2, 0)	- 2(2, 0)				[77039]
	98844.21	(0.10)	3(1, 0)	- 2(1, 0)			[77039]	
¹³ CH ₃ CD ₃	64352.89	(0.05)	2(1, 0)	- 1(1, 0)			[77039]	
	65006.83	(0.05)	2(1, 0)	- 1(1, 0)			[77039]	
CH ₃ ¹³ CD ₃ CH ₃ CHD ₂	34848.309	(0.050)	1(0, 1)	- 0(0, 0)	0	A	[79037]	
	34848.309	(0.050)	1(0, 1)	- 0(0, 0)	0	E	[79037]	
	69009.321	(0.050)	2(1, 2)	- 1(1, 1)	0	A	[79037]	
	69009.569	(0.050)	2(1, 2)	- 1(1, 1)	0	E	[79037]	
	69687.933	(0.050)	2(0, 2)	- 1(0, 1)	0	A	[79037]	
	69687.933	(0.050)	2(0, 2)	- 1(0, 1)	0	E	[79037]	
	70382.122	(0.050)	2(1, 1)	- 1(1, 0)	0	E	[79037]	
	70382.374	(0.050)	2(1, 1)	- 1(1, 0)	0	A	[79037]	
	78580.504	(0.050)	1(1, 0)	- 0(0, 0)	0	E	[79037]	
	78591.698	(0.050)	1(1, 0)	- 0(0, 0)	0	A	[79037]	
	103185.586	(0.050)	3(1, 3)	- 2(1, 2)	1	A	[81043]	
	103304.920	(0.050)	3(1, 3)	- 2(1, 2)	1	E	[81043]	
	103507.612	(0.050)	3(1, 3)	- 2(1, 2)	0	A	[79037]	
	103507.612	(0.050)	3(1, 3)	- 2(1, 2)	0	E	[79037]	
	104148.140	(0.050)	3(0, 3)	- 2(0, 2)	1	A	[81043]	
	104148.483	(0.050)	3(0, 3)	- 2(0, 2)	1	E	[81043]	
	104176.795	(0.050)	3(2, 2)	- 2(2, 1)	1	A	[81043]	
	104191.702	(0.050)	3(2, 2)	- 2(2, 1)	1	E	[81043]	
	104191.702	(0.050)	3(2, 1)	- 2(2, 0)	1	E	[81043]	
	104206.945	(0.050)	3(2, 1)	- 2(2, 0)	1	A	[81043]	
	104510.156	(0.050)	3(0, 3)	- 2(0, 2)	0	A	[79037]	
	104510.156	(0.050)	3(0, 3)	- 2(0, 2)	0	E	[79037]	
	104541.261	(0.050)	3(2, 2)	- 2(2, 1)	0	A	[79037]	
	104550.026	(0.050)	3(2, 2)	- 2(2, 1)	0	E	[79037]	
	104565.086	(0.050)	3(2, 1)	- 2(2, 0)	0	E	[79037]	
	104573.816	(0.050)	3(2, 1)	- 2(2, 0)	0	A	[79037]	
	105041.573	(0.050)	3(1, 2)	- 2(1, 1)	1	E	[81043]	
	105160.894	(0.050)	3(1, 2)	- 2(1, 1)	1	A	[81043]	
	105566.990	(0.050)	3(1, 2)	- 2(1, 1)	0	A	[79037]	
	105566.990	(0.050)	3(1, 2)	- 2(1, 1)	0	E	[79037]	
	114114.303	(0.050)	2(1, 1)	- 1(0, 1)	0	E	[79037]	
	114125.760	(0.050)	2(1, 1)	- 1(0, 1)	0	A	[79037]	
	114993.749	(0.050)	9(2, 8)	- 9(1, 8)	0	E	[79037]	
	115021.635	(0.050)	9(2, 8)	- 9(1, 8)	0	A	[79037]	
	117981.178	(0.050)	8(2, 7)	- 8(1, 7)	0	E	[79037]	
	118009.195	(0.050)	8(2, 7)	- 8(1, 7)	0	A	[79037]	
	120657.325	(0.050)	7(2, 6)	- 7(1, 6)	0	E	[79037]	
	120685.559	(0.050)	7(2, 6)	- 7(1, 6)	0	A	[79037]	
	123013.867	(0.050)	6(2, 5)	- 6(1, 5)	0	E	[79037]	
	123042.531	(0.050)	6(2, 5)	- 6(1, 5)	0	A	[79037]	
	125043.888	(0.050)	5(2, 4)	- 5(1, 4)	0	E	[79037]	
	125073.422	(0.050)	5(2, 4)	- 5(1, 4)	0	A	[79037]	
	126741.329	(0.050)	4(2, 3)	- 4(1, 3)	0	E	[79037]	
	126773.166	(0.050)	4(2, 3)	- 4(1, 3)	0	A	[79037]	
	128099.573	(0.050)	3(2, 2)	- 3(1, 2)	0	E	[79037]	
	128137.266	(0.050)	3(2, 2)	- 3(1, 2)	0	A	[79037]	
	129116.578	(0.050)	2(2, 1)	- 2(1, 1)	0	E	[79037]	
	129163.067	(0.050)	2(2, 1)	- 2(1, 1)	0	A	[79037]	
	137569.628	(0.050)	4(1, 4)	- 3(1, 3)	1	A	[81043]	
	137625.242	(0.050)	4(1, 4)	- 3(1, 3)	1	E	[81043]	
137998.215	(0.050)	4(1, 4)	- 3(1, 3)	0	A	[79037]		
137998.215	(0.050)	4(1, 4)	- 3(1, 3)	0	E	[79037]		
138826.507	(0.050)	4(0, 4)	- 3(0, 3)	1	A	[81043]		
138827.257	(0.050)	4(0, 4)	- 3(0, 3)	1	E	[81043]		
138893.987	(0.050)	4(2, 3)	- 3(2, 2)	1	A	[81043]		
138912.243	(0.050)	4(3, 2)	- 3(3, 1)	1	A	[81043]		
138912.243	(0.050)	4(3, 2)	- 3(3, 1)	1	E	[81043]		
138912.243	(0.050)	4(3, 1)	- 3(3, 0)	1	A	[81043]		
138912.243	(0.050)	4(3, 1)	- 3(3, 0)	1	E	[81043]		
138930.138	(0.050)	4(2, 3)	- 3(2, 2)	1	E	[81043]		
138932.294	(0.050)	4(2, 2)	- 3(2, 1)	1	E	[81043]		

TABLE 7.4. Microwave spectrum of ethane — Continued

C₂H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	v_1	Sym.	Vib. state	Ref.
CH ₃ CH ₂ D	138969.324	(0.050)	4(2, 2) - 3(2, 1)	1	A		[81043]
	139306.370	(0.050)	4(0, 4) - 3(0, 3)	0	A		[79037]
	139306.370	(0.050)	4(0, 4) - 3(0, 3)	0	E		[79037]
	139379.421	(0.050)	4(2, 3) - 3(2, 2)	0	A		[79037]
	139385.291	(0.050)	4(2, 3) - 3(2, 2)	0	E		[79037]
	139399.614	(0.050)	4(3, 2) - 3(3, 1)	0	A		[79037]
	139399.614	(0.050)	4(3, 2) - 3(3, 1)	0	E		[79037]
	139399.614	(0.050)	4(3, 1) - 3(3, 0)	0	A		[79037]
	139399.614	(0.050)	4(3, 1) - 3(3, 0)	0	E		[79037]
	139454.888	(0.050)	4(2, 2) - 3(2, 1)	0	E		[79037]
	139460.799	(0.050)	4(2, 2) - 3(2, 1)	0	A		[79037]
	140147.508	(0.050)	4(1, 3) - 3(1, 2)	1	E		[81043]
	140202.936	(0.050)	4(1, 3) - 3(1, 2)	1	A		[81043]
	140743.724	(0.050)	4(1, 3) - 3(1, 2)	0	A		[79037]
	140743.724	(0.050)	4(1, 3) - 3(1, 2)	0	E		[79037]
	110245.320	(0.050)	3(1, 3) - 2(1, 2)	0	A		[81034]
	110245.687	(0.050)	3(1, 3) - 2(1, 2)	0	E		[81034]
	111192.429	(0.050)	3(0, 3) - 2(0, 2)	0	A		[81034]
	111192.429	(0.050)	3(0, 3) - 2(0, 2)	0	E		[81034]
	111215.219	(0.050)	3(2, 2) - 2(2, 1)	0	A		[81034]
	111224.831	(0.050)	3(2, 2) - 2(2, 1)	0	E		[81034]
	111230.044	(0.050)	3(2, 1) - 2(2, 0)	0	E		[81034]
	111239.644	(0.050)	3(2, 1) - 2(2, 0)	0	A		[81034]
	112179.552	(0.050)	3(1, 2) - 2(1, 1)	0	E		[81034]
	112179.908	(0.050)	3(1, 2) - 2(1, 1)	0	A		[81034]
	124284.289	(0.050)	2(1, 2) - 1(0, 1)	0	E		[81034]
	124313.493	(0.050)	2(1, 2) - 1(0, 1)	0	A		[81034]
	141009.977	(0.050)	9(2, 7) - 9(1, 8)	0	E		[81034]
	141071.575	(0.050)	9(2, 7) - 9(1, 8)	0	A		[81034]
	143117.197	(0.050)	8(2, 6) - 8(1, 7)	0	E		[81034]
	143178.750	(0.050)	8(2, 6) - 8(1, 7)	0	A		[81034]
	145139.081	(0.050)	7(2, 5) - 7(1, 6)	0	E		[81034]
	145200.095	(0.050)	7(2, 5) - 7(1, 6)	0	A		[81034]
	146983.910	(0.050)	4(1, 4) - 3(1, 3)	0	A		[81034]
	146983.910	(0.050)	4(1, 4) - 3(1, 3)	0	E		[81034]
	147024.696	(0.050)	6(2, 4) - 6(1, 5)	0	E		[81034]
	147084.193	(0.050)	6(2, 4) - 6(1, 5)	0	A		[81034]
	148225.152	(0.050)	4(0, 4) - 3(0, 3)	0	A		[81034]
	148225.152	(0.050)	4(0, 4) - 3(0, 3)	0	E		[81034]
	148279.195	(0.050)	4(2, 3) - 3(2, 2)	0	A		[81034]
	148292.174	(0.050)	4(2, 3) - 3(2, 2)	0	E		[81034]
	148293.513	(0.050)	4(3, 2) - 3(3, 1)	0	A		[81034]
	148293.513	(0.050)	4(3, 2) - 3(3, 1)	0	E		[81034]
	148293.513	(0.050)	4(3, 1) - 3(3, 0)	0	A		[81034]
	148293.513	(0.050)	4(3, 1) - 3(3, 0)	0	E		[81034]
	148327.289	(0.050)	4(2, 2) - 3(2, 1)	0	E		[81034]
	148340.247	(0.050)	4(2, 2) - 3(2, 1)	0	A		[81034]
	148729.415	(0.050)	5(2, 3) - 5(1, 4)	0	E		[81034]
	148785.331	(0.050)	5(2, 3) - 5(1, 4)	0	A		[81034]
	149562.794	(0.050)	4(1, 3) - 3(1, 2)	0	A		[81034]
	149562.794	(0.050)	4(1, 3) - 3(1, 2)	0	E		[81034]
	150215.950	(0.050)	4(2, 2) - 4(1, 3)	0	E		[81034]
	150263.731	(0.050)	4(2, 2) - 4(1, 3)	0	A		[81034]
	151451.386	(0.050)	3(2, 1) - 3(1, 2)	0	E		[81034]
	151486.463	(0.050)	3(2, 1) - 3(1, 2)	0	A		[81034]
	152400.941	(0.050)	2(2, 0) - 2(1, 1)	0	E		[81034]
	152426.685	(0.050)	2(2, 0) - 2(1, 1)	0	A		[81034]
	154253.648	(0.050)	2(2, 1) - 2(1, 2)	0	E		[81034]
	154355.339	(0.050)	2(2, 1) - 2(1, 2)	0	A		[81034]
	155232.777	(0.050)	3(2, 2) - 3(1, 3)	0	E		[81034]
	155325.217	(0.050)	3(2, 2) - 3(1, 3)	0	A		[81034]
	156540.910	(0.050)	4(2, 3) - 4(1, 4)	0	E		[81034]
	156620.526	(0.050)	4(2, 3) - 4(1, 4)	0	A		[81034]
	158171.608	(0.050)	5(2, 4) - 5(1, 5)	0	E		[81034]
	158243.142	(0.050)	5(2, 4) - 5(1, 5)	0	A		[81034]
	160127.085	(0.050)	6(2, 5) - 6(1, 6)	0	E		[81034]
160194.865	(0.050)	6(2, 5) - 6(1, 6)	0	A		[81034]	

TABLE 7.4. Microwave spectrum of ethane — Continued

C₂H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_1	Sym.	Vib. state	Ref.
CD ₃ CH ₂ D	160390.374	(0.050)	3(1, 3) - 2(0, 2)	0	E		[81034]
	160419.313	(0.050)	3(1, 3) - 2(0, 2)	0	A		[81034]
	91852.580	(0.050)	3(1, 3) - 2(1, 2)	0	A		[81034]
	91852.580	(0.050)	3(1, 3) - 2(1, 2)	0	E		[81034]
	92500.262	(0.050)	3(0, 3) - 2(0, 2)	0	A		[81034]
	92500.262	(0.050)	3(0, 3) - 2(0, 2)	0	E		[81034]
	92516.865	(0.050)	3(2, 2) - 2(2, 1)	0	A		[81034]
	92517.476	(0.050)	3(2, 2) - 2(2, 1)	0	E		[81034]
	92533.862	(0.050)	3(2, 1) - 2(2, 0)	0	E		[81034]
	92534.498	(0.050)	3(2, 1) - 2(2, 0)	0	A		[81034]
	93177.102	(0.050)	3(1, 2) - 2(1, 1)	0	A		[81034]
	93177.102	(0.050)	3(1, 2) - 2(1, 1)	0	E		[81034]
	101934.857	(0.050)	4(2, 3) - 4(1, 4)	0	E		[81034]
	101941.912	(0.050)	4(2, 3) - 4(1, 4)	0	A		[81034]
	103046.424	(0.050)	5(2, 4) - 5(1, 5)	0	E		[81034]
	103053.458	(0.050)	5(2, 4) - 5(1, 5)	0	A		[81034]
	104383.724	(0.050)	6(2, 5) - 6(1, 6)	0	E		[81034]
	104390.734	(0.050)	6(2, 5) - 6(1, 6)	0	A		[81034]
	105948.419	(0.050)	7(2, 6) - 7(1, 7)	0	E		[81034]
	105955.410	(0.050)	7(2, 6) - 7(1, 7)	0	A		[81034]
	107742.159	(0.050)	8(2, 7) - 8(1, 8)	0	E		[81034]
	107749.188	(0.050)	8(2, 7) - 8(1, 8)	0	A		[81034]
	109766.725	(0.050)	9(2, 8) - 9(1, 9)	0	E		[81034]
	109773.713	(0.050)	9(2, 8) - 9(1, 9)	0	A		[81034]
	122463.143	(0.050)	4(1, 4) - 3(1, 3)	0	A		[81034]
	122463.143	(0.050)	4(1, 4) - 3(1, 3)	0	E		[81034]
	123311.192	(0.050)	4(0, 4) - 3(0, 3)	0	A		[81034]
	123311.192	(0.050)	4(0, 4) - 3(0, 3)	0	E		[81034]
	123350.492	(0.050)	4(2, 3) - 3(2, 2)	0	A		[81034]
	123350.492	(0.050)	4(2, 3) - 3(2, 2)	0	E		[81034]
	123361.047	(0.050)	4(3, 2) - 3(3, 1)	0	A		[81034]
	123361.047	(0.050)	4(3, 2) - 3(3, 1)	0	E		[81034]
	123361.047	(0.050)	4(3, 1) - 3(3, 0)	0	A		[81034]
	123361.047	(0.050)	4(3, 1) - 3(3, 0)	0	E		[81034]
	123394.328	(0.050)	4(2, 2) - 3(2, 1)	0	A		[81034]
	123394.328	(0.050)	4(2, 2) - 3(2, 1)	0	E		[81034]
	124228.913	(0.050)	4(1, 3) - 3(1, 2)	0	A		[81034]
	124228.913	(0.050)	4(1, 3) - 3(1, 2)	0	E		[81034]
	124434.724	(0.050)	3(1, 3) - 2(0, 2)	0	E		[81034]
	124439.121	(0.050)	3(1, 3) - 2(0, 2)	0	A		[81034]
	153067.769	(0.050)	5(1, 5) - 4(1, 4)	0	A		[81034]
	153067.769	(0.050)	5(1, 5) - 4(1, 4)	0	E		[81034]
	154102.907	(0.050)	5(0, 5) - 4(0, 4)	0	A		[81034]
	154102.907	(0.050)	5(0, 5) - 4(0, 4)	0	E		[81034]
	154179.349	(0.050)	5(2, 4) - 4(2, 3)	0	A		[81034]
	154179.349	(0.050)	5(2, 4) - 4(2, 3)	0	E		[81034]
	154194.108	(0.050)	5(4, 2) - 4(4, 1)	0	A		[81034]
154194.108	(0.050)	5(4, 2) - 4(4, 1)	0	E		[81034]	
154194.108	(0.050)	5(4, 1) - 4(4, 0)	0	A		[81034]	
154194.108	(0.050)	5(4, 1) - 4(4, 0)	0	E		[81034]	
154202.228	(0.050)	5(3, 3) - 4(3, 2)	0	E		[81034]	
154202.228	(0.050)	5(3, 2) - 4(3, 1)	0	E		[81034]	
154267.193	(0.050)	5(2, 3) - 4(2, 2)	0	A		[81034]	
154267.193	(0.050)	5(2, 3) - 4(2, 2)	0	E		[81034]	
154397.649	(0.050)	4(1, 4) - 3(0, 3)	0	E		[81034]	
154402.041	(0.050)	4(1, 4) - 3(0, 3)	0	A		[81034]	
155274.453	(0.050)	5(1, 4) - 4(1, 3)	0	A		[81034]	
155274.453	(0.050)	5(1, 4) - 4(1, 3)	0	E		[81034]	
g-CHDCH ₂ D	77445.640	(0.050)	13(1,12) - 13(0,13)	0	-		[81034]
	77446.349	(0.050)	13(1,12) - 13(0,13)	0	+		[81034]
	78396.638	(0.050)	1(1, 1) - 0(0, 0)	0	-		[81034]
	83467.019	(0.050)	14(1,13) - 14(0,14)	0	-		[81034]
	83467.878	(0.050)	14(1,13) - 14(0,14)	0	+		[81034]
	90105.326	(0.050)	15(1,14) - 15(0,15)	0	-		[81034]
	90106.333	(0.050)	15(1,14) - 15(0,15)	0	+		[81034]
	97365.259	(0.050)	16(1,15) - 16(0,16)	0	-		[81034]
	97366.416	(0.050)	16(1,15) - 16(0,16)	0	+		[81034]

TABLE 7.4. Microwave spectrum of ethane — Continued

C₂H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_1	Sym.	Vib. state	Ref.
	105241.651	(0.050)	17(1,16) - 17(0,17)	0	-		[81034]
	105242.991	(0.050)	17(1,16) - 17(0,17)	0	+		[81034]
	111276.929	(0.050)	15(2,13) - 15(1,14)	0			[81034]
	111350.322	(0.050)	19(2,17) - 19(0,18)	0			[81034]
	112290.034	(0.050)	14(2,12) - 14(1,13)	0			[81034]
	112469.187	(0.050)	2(1, 2) - 1(0, 1)	0			[81034]
	113607.607	(0.050)	13(2,11) - 13(1,12)	0			[81034]
	113719.162	(0.050)	18(1,17) - 18(0,18)	0	-		[81034]
	113720.660	(0.050)	18(1,17) - 18(0,18)	0	+		[81034]
	115169.134	(0.050)	12(2,10) - 12(1,11)	0			[81034]
	116912.078	(0.050)	11(2, 9) - 11(1, 0)	0			[81034]
	118773.025	(0.050)	10(2, 8) - 10(1, 9)	0			[81034]
	118993.973	(0.050)	7(1, 6) - 6(2, 5)	0			[81034]
	120689.399	(0.050)	9(2, 7) - 9(1, 8)	0			[81034]
	122600.827	(0.050)	8(2, 6) - 8(1, 7)	0			[81034]
	122772.194	(0.050)	19(1,18) - 19(0,18)	0	-		[81034]
	122773.891	(0.050)	19(1,18) - 19(0,18)	0	+		[81034]
	124450.640	(0.050)	7(2, 5) - 7(1, 6)	0			[81034]
	125856.511	(0.050)	10(2, 9) - 9(3, 6)	0			[81034]
	126186.723	(0.050)	6(2, 4) - 6(1, 5)	0			[81034]
	127762.620	(0.050)	5(2, 3) - 5(1, 4)	0			[81034]
	128920.627	(0.050)	10(2, 8) - 9(3, 7)	0			[81034]
	129138.004	(0.050)	4(2, 2) - 4(1, 3)	0			[81034]
	130278.990	(0.050)	3(2, 1) - 3(1, 2)	0			[81034]
	131158.466	(0.050)	2(2, 0) - 2(1, 1)	0			[81034]
	132182.656	(0.050)	5(0, 5) - 4(1, 4)	0			[81034]
	132967.054	(0.050)	2(2, 1) - 2(1, 2)	0			[81034]
	133464.872	(0.050)	8(1, 8) - 7(2, 5)	0			[81034]
	133877.339	(0.050)	3(2, 2) - 3(1, 3)	0			[81034]
	135093.274	(0.050)	4(2, 3) - 4(1, 4)	0			[81034]
	136616.765	(0.050)	5(2, 4) - 5(1, 5)	0			[81034]
	138449.877	(0.050)	6(2, 5) - 6(1, 6)	0			[81034]
	140594.707	(0.050)	7(2, 6) - 7(1, 7)	0			[81034]
	143053.896	(0.050)	8(2, 7) - 8(1, 8)	0			[81034]
	145829.764	(0.050)	9(2, 8) - 9(1, 9)	0	-		[81034]
	145830.070	(0.050)	9(2, 8) - 9(1, 9)	0	+		[81034]
	146240.402	(0.050)	3(1, 3) - 2(0, 2)	0			[81034]
	148924.720	(0.050)	10(2, 9) - 10(1,10)	0	-		[81034]
	148925.091	(0.050)	10(2, 9) - 10(1,10)	0	+		[81034]
	152340.534	(0.050)	11(2,10) - 11(1,11)	0	-		[81034]
	152340.972	(0.050)	11(2,10) - 11(1,11)	0	+		[81034]
	155994.334	(0.050)	8(1, 7) - 7(2, 6)	0			[81034]
	156078.768	(0.050)	12(2,11) - 12(1,12)	0	-		[81034]
	156079.256	(0.050)	12(2,11) - 12(1,12)	0	+		[81034]
	160140.430	(0.050)	13(2,12) - 13(1,13)	0	-		[81034]
	160141.073	(0.050)	13(2,12) - 13(1,13)	0	+		[81034]

Table 8.1. Molecular constants of CCCH in the X²Π state. [86010]

Parameter	CCCH
A _{eff} (MHz)	430828.(41)
B (MHz)	11186.335(2)
D x 10 ³ (MHz)	5.55(2)
γ _{eff} (MHz)	36.9(11)
p (MHz)	-7.20(7)
q (MHz)	-16.62(3)
P _D x 10 ³ (MHz)	47.4(24)
q _D x 10 ³ (MHz)	1.6(6)
P _H x 10 ⁶ (MHz)	45.(6)
q _H x 10 ⁶ (MHz)	3.1(21)
a (MHz)	12.3(2)
b + $\frac{c}{3}$ (MHz)	-13.8(6)
c (MHz)	28.3(14)
d (MHz)	16.2(1)

Table 8.2. Molecular Constants of the c-C₃H Radical. [87005]

Parameter	c-C ₃ H	Parameter	c-C ₃ H
A (MHz)	44536.840(50) ^a	ε _{aa} (MHz)	113.213(41) ^a
B (MHz)	34016.349(28)	ε _{bb} (MHz)	59.226(33)
C (MHz)	19188.8540(109)	ε _{cc} (MHz)	-205.808(35)
Δ _N (MHz)	0.05556(34)	a _F (MHz)	-27.270(72)
Δ _{NK} (MHz)	0.58832(86)	T _{aa} (MHz)	16.96(22)
Δ _K (MHz)	-0.4153(44)	T _{bb} (MHz)	-1.12(31)
δ _N (MHz)	0.020994(174)		
δ _K (MHz)	0.35928(121)		

^a The numbers in parentheses represent three standard deviations in units of the last significant digits.

TABLE 8.3. Microwave spectrum of ℓ -C₃H radicalC₃H

Isotopic species	Frequency (MHz)	Unc. (MHz)	J' - J''	P	F' - F''	Vib. state	Ref.	
ℓ -C ₃ H $^2\Pi_{1/2}$	32627.300	(0.05)	3/2 - 1/2	<i>a</i>	2 - 1	$\nu = 0$	[86010]	
	32634.390	(0.05)	3/2 - 1/2	<i>a</i>	1 - 0	$\nu = 0$	[86010]	
	32660.655	(0.05)	3/2 - 1/2	<i>b</i>	2 - 1	$\nu = 0$	[86010]	
	32663.375	(0.05)	3/2 - 1/2	<i>b</i>	1 - 0	$\nu = 0$	[86010]	
	97995.166	(0.05)	9/2 - 7/2	<i>b</i>	5 - 4	$\nu = 0$	[85006]	
	97995.913	(0.05)	9/2 - 7/2	<i>b</i>	4 - 3	$\nu = 0$	[85006]	
	98011.611	(0.05)	9/2 - 7/2	<i>a</i>	5 - 4	$\nu = 0$	[85006]	
	98012.524	(0.05)	9/2 - 7/2	<i>a</i>	4 - 3	$\nu = 0$	[85006]	
	119804.682	(0.05)	11/2 - 9/2	<i>b</i>	6 - 5	$\nu = 0$	[85006]	
	119805.322	(0.05)	11/2 - 9/2	<i>b</i>	5 - 4	$\nu = 0$	[85006]	
	119847.476	(0.05)	11/2 - 9/2	<i>a</i>	6 - 5	$\nu = 0$	[85006]	
	119858.259	(0.05)	11/2 - 9/2	<i>a</i>	5 - 4	$\nu = 0$	[85006]	
	141635.793	(0.05)	13/2 - 11/2	<i>a</i>	7 - 6	$\nu = 0$	[85006]	
	141636.431	(0.05)	13/2 - 11/2	<i>a</i>	6 - 5	$\nu = 0$	[85006]	
	141708.728	(0.05)	13/2 - 11/2	<i>a</i>	7 - 6	$\nu = 0$	[85006]	
	141709.494	(0.05)	13/2 - 11/2	<i>a</i>	6 - 5	$\nu = 0$	[85006]	
	163491.035	(0.05)	15/2 - 13/2	<i>a</i>	8 - 7	$\nu = 0$	[85006]	
	163491.557	(0.05)	15/2 - 13/2	<i>a</i>	7 - 6	$\nu = 0$	[85006]	
	163597.232	(0.05)	15/2 - 13/2	<i>b</i>	8 - 7	$\nu = 0$	[85006]	
	163597.900	(0.05)	15/2 - 13/2	<i>b</i>	7 - 6	$\nu = 0$	[85006]	
	185371.952	(0.05)	17/2 - 15/2	<i>a</i>	9 - 8	$\nu = 0$	[85006]	
	185372.417	(0.05)	17/2 - 15/2	<i>a</i>	8 - 7	$\nu = 0$	[85006]	
	185513.968	(0.05)	17/2 - 15/2	<i>b</i>	9 - 8	$\nu = 0$	[85006]	
	185514.589	(0.05)	17/2 - 15/2	<i>b</i>	8 - 7	$\nu = 0$	[85006]	
	ℓ -C ₃ H $^2\Pi_{3/2}$	80388.107	(0.05)	7/2 - 5/2	<i>a</i>	4 - 3	$\nu = 0$	[85006]
		80389.442	(0.05)	7/2 - 5/2	<i>a</i>	3 - 2	$\nu = 0$	[85006]
		80420.646	(0.05)	7/2 - 5/2	<i>b</i>	4 - 3	$\nu = 0$	[85006]
		80422.052	(0.05)	7/2 - 5/2	<i>b</i>	3 - 2	$\nu = 0$	[85006]
		80422.052	(0.05)	7/2 - 5/2	<i>b</i>	3 - 2	$\nu = 0$	[85006]
		103319.276	(0.05)	9/2 - 7/2	<i>a</i>	5 - 4	$\nu = 0$	[85006]
		103319.786	(0.05)	9/2 - 7/2	<i>a</i>	4 - 3	$\nu = 0$	[85006]
		103372.483	(0.05)	9/2 - 7/2	<i>b</i>	5 - 4	$\nu = 0$	[85006]
103373.094		(0.05)	9/2 - 7/2	<i>b</i>	4 - 3	$\nu = 0$	[85006]	
149106.972		(0.05)	13/2 - 11/2	<i>a</i>	6 - 5	$\nu = 0$	[85006]	
149106.972		(0.05)	13/2 - 11/2	<i>a</i>	7 - 6	$\nu = 0$	[85006]	
149212.667		(0.05)	13/2 - 11/2	<i>b</i>	6 - 5	$\nu = 0$	[85006]	
149212.667		(0.05)	13/2 - 11/2	<i>b</i>	7 - 6	$\nu = 0$	[85006]	
171958.650		(0.05)	15/2 - 13/2	<i>a</i>	7 - 6	$\nu = 0$	[85006]	
171958.650		(0.05)	15/2 - 13/2	<i>a</i>	8 - 7	$\nu = 0$	[85006]	
172094.778		(0.05)	15/2 - 13/2	<i>b</i>	8 - 7	$\nu = 0$	[85006]	
172094.778		(0.05)	15/2 - 13/2	<i>b</i>	7 - 6	$\nu = 0$	[85006]	
194780.373		(0.05)	17/2 - 15/2	<i>a</i>	8 - 7	$\nu = 0$	[85006]	
194780.373		(0.05)	17/2 - 15/2	<i>a</i>	9 - 8	$\nu = 0$	[85006]	
194948.795		(0.05)	17/2 - 15/2	<i>b</i>	8 - 7	$\nu = 0$	[85006]	
194948.795		(0.05)	17/2 - 15/2	<i>b</i>	9 - 8	$\nu = 0$	[85006]	

TABLE 8.4. Microwave spectrum of cyclic-C₃H radicalC₃H

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	$F' F'_1 - F'' F''_1$	Ref.
CCHC □	91494.349	(0.030)	2(1, 2) - 1(1, 1)	5/2 3 - 3/2 2	[87005]
	91497.608	(0.030)	2(1, 2) - 1(1, 1)	5/2 2 - 3/2 2	[87005]
H C / \ C-C	91692.752	(0.030)	2(1, 2) - 1(1, 1)	3/2 1 - 1/2 0	[87005]
	91699.471	(0.030)	2(1, 2) - 1(1, 1)	3/2 2 - 1/2 1	[87005]
	121211.689	(0.030)	2(1, 1) - 1(1, 0)	5/2 3 - 3/2 2	[87005]
	121213.226	(0.030)	2(1, 1) - 1(1, 0)	5/2 2 - 3/2 1	[87005]
	216488.036	(0.030)	4(1, 3) - 3(1, 2)	9/2 5 - 7/2 4	[87005]
	216492.396	(0.030)	4(1, 3) - 3(1, 2)	9/2 4 - 7/2 3	[87005]
	216638.026	(0.030)	4(1, 3) - 3(1, 2)	7/2 4 - 5/2 3	[87005]
	216640.873	(0.030)	4(1, 3) - 3(1, 2)	7/2 3 - 5/2 2	[87005]
	223301.273	(0.030)	4(3, 2) - 3(3, 1)	9/2 5 - 7/2 4	[87005]
	223304.238	(0.030)	4(3, 2) - 3(3, 1)	9/2 4 - 7/2 3	[87005]
	223439.668	(0.030)	4(3, 2) - 3(3, 1)	7/2 3 - 5/2 2	[87005]
	223444.640	(0.030)	4(3, 2) - 3(3, 1)	7/2 4 - 5/2 3	[87005]
	238636.443	(0.030)	4(3, 1) - 3(3, 0)	9/2 5 - 7/2 4	[87005]
	238638.558	(0.030)	4(3, 1) - 3(3, 0)	9/2 4 - 7/2 3	[87005]
	238686.633	(0.030)	4(3, 1) - 3(3, 0)	7/2 3 - 5/2 2	[87005]
	238692.077	(0.030)	4(3, 1) - 3(3, 0)	7/2 4 - 5/2 3	[87005]
	249544.254	(0.030)	6(1, 6) - 5(1, 5)	13/2 7 - 11/2 6	[87005]
	249544.254	(0.030)	6(1, 6) - 5(1, 5)	13/2 6 - 11/2 5	[87005]
	249746.796	(0.030)	6(1, 6) - 5(1, 5)	11/2 6 - 9/2 5	[87005]
	249746.796	(0.030)	6(1, 6) - 5(1, 5)	11/2 5 - 9/2 4	[87005]
	287920.669	(0.030)	7(1, 7) - 6(1, 6)	15/2 8 - 13/2 7	[87005]
	287920.669	(0.030)	7(1, 7) - 6(1, 6)	15/2 7 - 13/2 6	[87005]
	288124.063	(0.030)	7(1, 7) - 6(1, 6)	13/2 7 - 11/2 6	[87005]
	288124.063	(0.030)	7(1, 7) - 6(1, 6)	13/2 6 - 11/2 5	[87005]
	326286.929	(0.030)	8(1, 8) - 7(1, 7)	17/2 9 - 15/2 8	[87005]
	326286.929	(0.030)	8(1, 8) - 7(1, 7)	17/2 8 - 15/2 7	[87005]
	326490.831	(0.030)	8(1, 8) - 7(1, 7)	15/2 8 - 13/2 7	[87005]
	326490.831	(0.030)	8(1, 8) - 7(1, 7)	15/2 7 - 13/2 6	[87005]

Table 9.1. Molecular constants for cyclopropenylidene (HCCCH).

Parameter	Value [present]	Parameter	Value [86008]
A'' (MHz)	35092.5923(56) ^a	A (MHz)	35092.6121(18) ^b
B'' (MHz)	32212.9250(56)	B (MHz)	32212.7811(18)
C'' (MHz)	16749.3081(56)	C (MHz)	16749.1067(18)
τ_1 (MHz)	-0.6762(14)	D _J (MHz)	0.020307(37)
τ_2 (MHz)	-0.16277(46)	D _{JK} (MHz)	0.1720642(25)
τ_3 (MHz)	17.314(14)	D _K (MHz)	-0.0448652(41)
τ_{aaaa} (MHz)	-0.59028(46)	d ₁ (MHz)	-0.0163698(14)
τ_{bbbb} (MHz)	-0.29821(46)	d ₂ (MHz)	-0.01070597(70)
τ_{cccc} (MHz)	-0.03548(48)	H _J (Hz)	0 ^c
H _J (Hz)	0 ^c	H _{JK} (Hz)	3.2560(22)
H _{JK} (Hz)	4.388(17)	H _{KJ} (Hz)	-9.359(16)
H _{KJ} (Hz)	-11.747(110)	H _K (Hz)	7.288(28)
H _K (Hz)	8.716(101)	h ₁ (Hz)	0 ^c
h _J (Hz)	0.609(26)	h ₂ (Hz)	0.16144(68)
h _{JK} (Hz)	0 ^c	h ₃ (Hz)	0 ^c
h _K (Hz)	0.461(57)	L _{JK} (Hz)	-0.000126(19)
		L _K (Hz)	0.000292(38)
σ^d	1.4	σ^e (kHz)	19.2

Electric Dipole Moment

μ (D)	3.32(5) [87011]
	3.43(2) [87022]

^aTwo standard deviations.^bOne standard deviation.^cThese constants were poorly determined and set to zero.^dWeighted fit. This gives a standard deviation of about 30 kHz.^eUnweighted fit.

Table 9.2. Molecular constants for cyclopropenylidene and its monosubstituted derivatives. [87004]

Parameter	C ₃ H ₂	¹³ C on-axis	¹³ C off-axis	C ₃ HD
A (MHz)	35092.5083(32) ^a	33310.5202(50)	34857.1875(25)	34517.5188(16)
B (MHz)	32212.9468(32)	32212.5804(43)	31288.4887(24)	26965.8135(15)
C (MHz)	16749.0286(32)	16331.2875(27)	16443.0399(22)	15098.4567(12)
Δ _J (kHz)	41.689(65)	41.482(45)	40.338(35)	30.892(13)
Δ _{JK} (kHz)	44.017(55)	36.618(89)	38.941(26)	51.623(20)
Δ _K (kHz)	61.871(38)	53.679(99)	65.734(21)	61.068(24)
δ _J (kHz)	16.4338(86)	16.5134(81)	15.9455(40)	12.0039(38)
δ _K (kHz)	58.610(20)	53.155(20)	56.422(10)	60.265(11)
H _J (Hz)	0 ^b	0 ^b	0 ^b	0 ^b
H _{JK} (Hz)	6.37(84)	5.53(26)	5.268(18)	2.405(44)
H _{KJ} (Hz)	-14.7(12)	-14.32(49)	-11.019(28)	-4.39(16)
H _K (Hz)	10.08(56)	9.94(30)	7.319(44)	2.66(20)
h _J (Hz)	0.477(75)	0.477 ^c	0.477 ^c	0.2225(73)
h _{JK} (Hz)	-0.88(37)	-0.88 ^c	-0.88 ^c	-0.88 ^c
h _K (Hz)	1.22(31)	1.22 ^c	1.22 ^c	3.706(88)
σ (kHz) ^d	34.1	37.6	26.7	28.3
eQq _{aa} (kHz) ^e				180.9(13)
eQq _{cc} (kHz) ^e				-87.5(18)

^aThe numbers in parentheses denote one standard deviation in the last quoted digits.

^bThis constant was set equal to zero.

^cThese constants were constrained to the values obtained for the parent species.

^dStandard deviation of the fit.

^eReference [87016].

TABLE 9.3. Microwave spectrum of cyclopropenylidene

C₃H₂

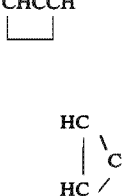
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	$F' - F''$	Ref.
CHCCH	18343.145	(0.002)	1(1, 0) - 1(0, 1)		[85018]
	46755.620	(0.020)	2(1, 1) - 2(0, 2)		[84034]
	85338.89	(0.02)	2(1, 2) - 1(0, 1)		[85019]
	118382.174	(0.020)	8(6, 3) - 8(5, 4)		[86008]
	119077.949	(0.020)	17(14, 3) - 17(13, 4)		[86008]
	119959.163	(0.020)	9(7, 3) - 9(6, 4)		[86008]
	121791.957	(0.020)	21(16, 5) - 21(15, 6)		[86008]
	122023.482	(0.020)	2(2, 1) - 1(1, 0)		[86008]
	122642.058	(0.020)	12(11, 1) - 12(10, 2)		[86008]
	122668.503	(0.020)	10(8, 3) - 10(7, 4)		[86008]
	123879.216	(0.020)	20(15, 5) - 20(14, 6)		[86008]
	124528.888	(0.020)	22(17, 5) - 22(16, 6)		[86008]
	125076.446	(0.020)	20(16, 4) - 20(15, 5)		[86008]
	129904.589	(0.020)	19(14, 5) - 19(13, 6)		[86008]
	130924.250	(0.020)	10(10, 1) - 10(9, 2)		[86008]
	131444.599	(0.020)	15(13, 2) - 15(12, 3)		[86008]
	132381.515	(0.020)	12(10, 3) - 12(9, 4)		[86008]
	132481.568	(0.020)	23(18, 5) - 23(17, 6)		[86008]
	133675.079	(0.020)	12(8, 4) - 12(7, 5)		[86008]
	137243.878	(0.020)	18(15, 3) - 18(14, 4)		[86008]
	138548.221	(0.020)	18(13, 5) - 18(12, 6)		[86008]
	138566.055	(0.020)	12(11, 2) - 12(10, 3)		[86008]
	150820.660	(0.030)	4(0, 4) - 3(1, 3)		[85019]
	150851.910	(0.020)	4(1, 4) - 3(0, 3)		[85019]
	162562.513	(0.020)	16(13, 4) - 16(12, 5)		[86008]
	162874.252	(0.020)	25(20, 5) - 25(19, 6)		[86008]
	164391.465	(0.020)	14(13, 2) - 14(12, 3)		[86008]
	165176.294	(0.020)	28(22, 6) - 28(21, 7)		[86008]
	165492.391	(0.020)	15(10, 5) - 15(9, 6)		[86008]
	165884.284	(0.080)	5(5, 0) - 5(2, 3)		[86008]
	167134.630	(0.080)	27(20, 7) - 27(19, 8)		[86008]
	169424.718	(0.020)	21(15, 6) - 21(14, 7)		[86008]
	169483.646	(0.020)	17(15, 2) - 17(14, 3)		[86008]
	169546.654	(0.040)	31(24, 7) - 31(23, 8)		[86008]
	169748.773	(0.040)	17(14, 4) - 17(13, 5)		[86008]
	170229.482	(0.020)	16(14, 3) - 16(13, 4)		[86008]
	171617.071	(0.030)	14(9, 5) - 14(8, 6)		[86008]
	172314.030	(0.020)	13(13, 0) - 13(12, 1)		[86008]
173186.951	(0.020)	13(13, 1) - 13(12, 2)		[86008]	
174100.976	(0.020)	15(14, 1) - 15(13, 2)		[86008]	
174690.832	(0.050)	33(25, 8) - 33(24, 9)		[86008]	
176039.531	(0.020)	13(8, 5) - 13(7, 6)		[86008]	
177395.468	(0.120)	5(3, 3) - 4(4, 0)		[86008]	
177413.211	(0.100)	32(24, 8) - 32(23, 9)		[86008]	
177436.348	(0.020)	20(17, 3) - 20(16, 4)		[86008]	
177645.831	(0.030)	26(19, 7) - 26(18, 8)		[86008]	
177754.508	(0.080)	6(6, 0) - 6(3, 3)		[86008]	
177792.301	(0.050)	34(26, 8) - 34(25, 9)		[86008]	
178197.398	(0.020)	15(14, 2) - 15(13, 3)		[86008]	
178426.066	(0.020)	15(11, 5) - 15(10, 6)		[86008]	
178543.316	(0.020)	18(15, 4) - 18(14, 5)		[86008]	
178569.558	(0.020)	16(12, 5) - 16(11, 6)		[86008]	
178952.041	(0.020)	14(10, 5) - 14(9, 6)		[86008]	
179105.811	(0.020)	12(7, 5) - 12(6, 6)		[86008]	
179682.002	(0.020)	17(13, 5) - 17(12, 6)		[86008]	
179867.006	(0.020)	13(9, 5) - 13(8, 6)		[86008]	
180279.516	(0.020)	20(14, 6) - 20(13, 7)		[86008]	
180938.024	(0.020)	12(8, 5) - 12(7, 6)		[86008]	
181196.922	(0.020)	11(6, 5) - 11(5, 6)		[86008]	
181786.979	(0.020)	23(19, 4) - 23(18, 5)		[86008]	
181995.810	(0.020)	11(7, 5) - 11(6, 6)		[86008]	
182045.875	(0.020)	18(14, 5) - 18(13, 6)		[86008]	
182622.910	(0.020)	10(5, 5) - 10(4, 6)		[86008]	
182770.880	(0.020)	17(15, 3) - 17(14, 4)		[86008]	
182936.042	(0.020)	10(6, 5) - 10(5, 6)		[86008]	
183338.773	(0.020)	26(21, 5) - 26(20, 6)		[86008]	
183464.869	(0.030)	29(23, 6) - 29(22, 7)		[86008]	

TABLE 9.3. Microwave spectrum of cyclopropenylidene — Continued

C₃H₂

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	$F' - F''$	Ref.
	183601.776	(0.020)	9(4, 5) - 9(3, 6)		[86008]
	183623.622	(0.020)	4(1, 3) - 3(2, 2)		[86008]
	183709.794	(0.020)	9(5, 5) - 9(4, 6)		[86008]
	183993.055	(0.050)	32(25, 7) - 32(24, 8)		[86008]
	184276.268	(0.020)	8(3, 5) - 8(2, 6)		[86008]
	184307.984	(0.020)	8(4, 5) - 8(3, 6)		[86008]
	184327.934	(0.020)	5(0, 5) - 4(1, 4)		[86008]
	184329.985	(0.020)	5(1, 5) - 4(0, 4)		[86008]
	184738.130	(0.020)	7(2, 5) - 7(1, 6)		[86008]
	184745.527	(0.020)	7(3, 5) - 7(2, 6)		[86008]
	185047.698	(0.020)	6(1, 5) - 6(0, 6)		[86008]
	185049.024	(0.020)	6(2, 5) - 6(1, 6)		[86008]
	185126.066	(0.020)	31(23, 8) - 31(22, 9)		[86008]
	185617.510	(0.020)	4(2, 3) - 3(1, 2)		[86008]
	185891.212	(0.020)	19(15, 5) - 19(14, 6)		[86008]
	186964.477	(0.050)	35(27, 8) - 35(26, 9)		[86008]
	187118.237	(0.020)	14(14, 0) - 14(13, 1)		[86008]
	187499.640	(0.020)	18(16, 2) - 18(15, 3)		[86008]
	187589.020	(0.020)	14(14, 1) - 14(13, 2)		[86008]
	193488.758	(0.020)	3(3, 1) - 2(2, 0)		[86008]
	194645.051	(0.100)	7(7, 0) - 7(4, 3)		[86008]
	196083.755	(0.020)	18(16, 3) - 18(15, 4)		[86008]
	196472.035	(0.080)	30(22, 8) - 30(21, 9)		[86008]
	197215.611	(0.020)	21(18, 3) - 21(17, 4)		[86008]
	197512.295	(0.020)	18(12, 6) - 18(11, 7)		[86008]
	198525.779	(0.020)	21(17, 5) - 21(16, 6)		[86008]
	200362.725	(0.020)	20(17, 4) - 20(16, 5)		[86008]
	201783.140	(0.020)	15(15, 0) - 15(14, 1)		[86008]
	202032.489	(0.020)	15(15, 1) - 15(14, 2)		[86008]
	202093.595	(0.020)	24(17, 7) - 24(16, 8)		[86008]
	202894.654	(0.060)	35(26, 9) - 35(25, 10)		[86008]
	203034.961	(0.080)	33(26, 7) - 33(25, 8)		[86008]
	203102.564	(0.030)	24(20, 4) - 24(19, 5)		[86008]
	203340.626	(0.020)	17(11, 6) - 17(10, 7)		[86008]
	204611.028	(0.030)	19(17, 2) - 19(16, 3)		[86008]
	204788.926	(0.030)	4(2, 2) - 3(3, 1)		[86008]
	205313.470	(0.020)	17(16, 1) - 17(15, 2)		[86008]
	205387.990	(0.020)	27(22, 5) - 27(21, 6)		[86008]
	206686.948	(0.020)	17(16, 2) - 17(15, 3)		[86008]
	206744.224	(0.020)	20(15, 6) - 20(14, 7)		[86008]
	206879.581	(0.020)	19(14, 6) - 19(13, 7)		[86008]
	207318.462	(0.020)	22(18, 5) - 22(17, 6)		[86008]
	207609.734	(0.020)	16(10, 6) - 16(9, 7)		[86008]
	207644.919	(0.020)	21(16, 6) - 21(15, 7)		[86008]
	207753.464	(0.020)	18(13, 6) - 18(12, 7)		[86008]
	238572.986	(0.060)	21(19, 3) - 21(18, 4)		[86008]
	238976.748	(0.020)	19(12, 7) - 19(11, 8)		[86008]
	240245.969	(0.040)	23(20, 4) - 23(19, 5)		[86008]
	241250.040	(0.030)	19(13, 7) - 19(12, 8)		[86008]
	242076.807	(0.030)	18(11, 7) - 18(10, 8)		[86008]
	243204.340	(0.020)	18(12, 7) - 18(11, 8)		[86008]
	244461.198	(0.020)	17(10, 7) - 17(9, 8)		[86008]
	244988.078	(0.020)	17(11, 7) - 17(10, 8)		[86008]
	245358.580	(0.030)	18(18, 1) - 18(17, 2)		[86008]
	245627.243	(0.050)	28(22, 7) - 28(21, 8)		[86008]
	246326.853	(0.050)	16(9, 7) - 16(8, 8)		[86008]
	246557.769	(0.020)	16(10, 7) - 16(9, 8)		[86008]
	247807.193	(0.020)	15(8, 7) - 15(7, 8)		[86008]
	247901.483	(0.020)	15(9, 7) - 15(8, 8)		[86008]
	248991.700	(0.020)	14(7, 7) - 14(6, 8)		[86008]
	249027.195	(0.020)	14(8, 7) - 14(7, 8)		[86008]
	249045.831	(0.080)	29(24, 5) - 29(23, 6)		[86008]
	249054.368	(0.020)	5(2, 3) - 4(3, 2)		[86008]
	249888.758	(0.060)	20(19, 1) - 20(18, 2)		[86008]
	249941.555	(0.020)	13(6, 7) - 13(5, 8)		[86008]
	249953.727	(0.020)	13(7, 7) - 13(6, 8)		[86008]
	250116.834	(0.050)	20(19, 2) - 20(18, 3)		[86008]

TABLE 9.3. Microwave spectrum of cyclopropenylidene — Continued

C₃H₂

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	$F' - F''$	Ref.
	250700.606	(0.020)	12(5, 7) - 12(4, 8)		[86008]
	250704.357	(0.020)	12(6, 7) - 12(5, 8)		[86008]
	260479.746	(0.020)	5(3, 2) - 4(4, 1)		[86008]
	262387.197	(0.030)	26(19, 8) - 26(18, 9)		[86008]
	262567.100	(0.060)	30(23, 8) - 30(22, 9)		[86008]
	264467.138	(0.030)	21(20, 1) - 21(19, 2)		[86008]
	265759.438	(0.030)	4(4, 1) - 3(3, 0)		[86008]
	266190.313	(0.030)	23(15, 8) - 23(14, 9)		[86008]
	266639.231	(0.030)	25(22, 3) - 25(21, 4)		[86008]
	266867.115	(0.030)	24(17, 8) - 24(16, 9)		[86008]
	270127.641	(0.030)	22(14, 8) - 22(13, 9)		[86008]
	271795.226	(0.030)	22(15, 8) - 22(14, 9)		[86008]
	273235.958	(0.050)	21(13, 8) - 21(12, 9)		[86008]
	274071.906	(0.050)	21(14, 8) - 21(13, 9)		[86008]
	274144.163	(0.120)	20(20, 1) - 20(19, 2)		[86008]
	275734.555	(0.080)	20(12, 8) - 20(11, 9)		[86008]
	276133.083	(0.050)	20(13, 8) - 20(12, 9)		[86008]
	310861.584	(0.080)	21(12, 9) - 21(11,10)		[86008]
	312488.672	(0.080)	20(12, 9) - 20(11,10)		[86008]
	326152.758	(0.100)	6(4, 3) - 5(3, 2)		[86008]
	345373.745	(0.080)	22(13,10) - 22(12,11)		[86008]
	346732.212	(0.100)	21(11,10) - 21(10,11)		[86008]
	386218.136	(0.080)	8(4, 5) - 7(3, 4)		[86008]
	410296.084	(0.100)	6(6, 1) - 5(5, 0)		[86008]
CH ¹³ CCH	142698.170	(0.040)	15(11, 4) - 15(10, 5)		[87004]
	144839.149	(0.060)	18(15, 4) - 18(14, 5)		[87004]
	145060.711	(0.040)	16(13, 4) - 16(12, 5)		[87004]
	145148.239	(0.040)	13(9, 4) - 13(8, 5)		[87004]
	145353.129	(0.030)	3(1, 2) - 2(2, 1)		[87004]
	145501.597	(0.050)	20(17, 4) - 20(16, 5)		[87004]
	145705.463	(0.040)	14(11, 4) - 14(10, 5)		[87004]
	146490.725	(0.030)	11(7, 4) - 11(6, 5)		[87004]
	147026.576	(0.030)	10(7, 4) - 10(6, 5)		[87004]
	147069.698	(0.030)	4(1, 4) - 3(0, 3)		[87004]
	147201.828	(0.030)	9(5, 4) - 9(4, 5)		[87004]
	147255.449	(0.070)	9(6, 4) - 9(5, 5)		[87004]
	147436.085	(0.040)	8(5, 4) - 8(4, 5)		[87004]
	147565.703	(0.040)	7(3, 4) - 7(2, 5)		[87004]
	147671.722	(0.040)	6(3, 4) - 6(2, 5)		[87004]
	147739.746	(1.20)	5(1, 4) - 5(0, 5)		[87004]
	174781.357	(0.080)	19(14, 5) - 19(13, 6)		[87004]
	175607.464	(0.040)	20(16, 5) - 20(15, 6)		[87004]
	178091.994	(1.00)	16(12, 5) - 16(11, 6)		[87004]
	178423.923	(0.050)	15(10, 5) - 15(9, 6)		[87004]
	179013.395	(0.040)	14(10, 5) - 14(9, 6)		[87004]
	179337.748	(0.050)	13(8, 5) - 13(7, 6)		[87004]
	179728.417	(0.040)	5(0, 5) - 4(1, 4)		[87004]
	179728.417	(0.040)	5(1, 5) - 4(0, 4)		[87004]
	179782.257	(0.080)	4(1, 3) - 3(2, 2)		[87004]
	179923.496	(1.20)	11(6, 5) - 11(5, 6)		[87004]
	180067.190	(0.040)	4(2, 3) - 3(1, 2)		[87004]
	180128.715	(0.080)	10(5, 5) - 10(4, 6)		[87004]
	180131.596	(0.030)	10(6, 5) - 10(5, 6)		[87004]
	180289.074	(0.030)	9(4, 5) - 9(3, 6)		[87004]
	180412.793	(0.030)	8(4, 5) - 8(3, 6)		[87004]
	180506.019	(0.080)	7(2, 5) - 7(1, 6)		[87004]
	180575.288	(0.080)	6(2, 5) - 6(1, 6)		[87004]
	210761.946	(0.050)	18(13, 6) - 18(12, 7)		[87004]
	211219.261	(0.050)	17(11, 6) - 17(10, 7)		[87004]
	211613.800	(0.050)	3(3, 0) - 2(2, 1)		[87004]
	211649.403	(1.00)	16(10, 6) - 16(9, 7)		[87004]
	212014.497	(0.050)	15(9, 6) - 15(8, 7)		[87004]
	212020.063	(1.00)	15(10, 6) - 15(9, 7)		[87004]
	212322.747	(0.080)	14(8, 6) - 14(7, 7)		[87004]
	212325.189	(0.040)	14(9, 6) - 14(8, 7)		[87004]
	212387.110	(0.030)	6(0, 6) - 5(1, 5)		[87004]
	212387.110	(0.030)	6(1, 6) - 5(0, 5)		[87004]

TABLE 9.3. Microwave spectrum of cyclopropenylidene — Continued

C₃H₂

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	$F' - F''$	Ref.
	212563.331	(0.030)	5(1, 4) - 4(2, 3)		[87004]
	212575.631	(0.070)	5(2, 4) - 4(1, 3)		[87004]
	212581.455	(0.030)	13(7, 6) - 13(6, 7)		[87004]
	212797.375	(0.030)	12(7, 6) - 12(6, 7)		[87004]
	212975.143	(0.050)	11(5, 6) - 11(4, 7)		[87004]
	213120.737	(0.030)	10(5, 6) - 10(4, 7)		[87004]
	213238.520	(0.050)	9(3, 6) - 9(2, 7)		[87004]
	213332.649	(0.080)	8(3, 6) - 8(2, 7)		[87004]
	216083.568	(0.030)	4(3, 2) - 3(2, 1)		[87004]
	244920.515	(0.080)	16(10, 7) - 16(9, 8)		[87004]
	245040.632	(0.070)	5(2, 3) - 4(3, 2)		[87004]
	245044.421	(0.070)	7(0, 7) - 6(1, 6)		[87004]
	245044.421	(0.070)	7(1, 7) - 6(0, 6)		[87004]
	245189.410	(0.080)	15(8, 7) - 15(7, 8)		[87004]
	245421.364	(1.00)	14(8, 7) - 14(7, 8)		[87004]
	245789.540	(1.00)	12(6, 7) - 12(5, 8)		[87004]
	245932.686	(0.050)	11(4, 7) - 11(3, 8)		[87004]
¹³ CHCCCH	119816.200	(0.040)	19(14, 5) - 19(13, 6)		[87004]
	120566.004	(0.040)	18(13, 5) - 18(12, 6)		[87004]
	120893.908	(0.030)	9(7, 3) - 9(6, 4)		[87004]
	122458.091	(0.040)	13(11, 2) - 13(10, 3)		[87004]
	125373.048	(0.030)	20(15, 5) - 20(14, 6)		[87004]
	141276.758	(0.030)	9(5, 4) - 9(4, 5)		[87004]
	141368.878	(0.030)	11(10, 2) - 11(9, 3)		[87004]
	141482.632	(0.030)	12(10, 3) - 12(9, 4)		[87004]
	143766.071	(0.030)	14(12, 2) - 14(11, 3)		[87004]
	144662.801	(0.030)	8(4, 4) - 8(3, 5)		[87004]
	145767.604	(0.040)	19(15, 4) - 19(14, 5)		[87004]
	146087.730	(0.030)	10(7, 4) - 10(6, 5)		[87004]
	146179.089	(0.040)	9(6, 4) - 9(5, 5)		[87004]
	146669.928	(0.030)	7(3, 4) - 7(2, 5)		[87004]
	146719.675	(0.030)	8(5, 4) - 8(4, 5)		[87004]
	146838.483	(0.030)	15(10, 5) - 15(9, 6)		[87004]
	146841.283	(0.030)	11(8, 4) - 11(7, 5)		[87004]
	147398.181	(0.040)	7(4, 4) - 7(3, 5)		[87004]
	147483.771	(0.040)	12(11, 1) - 12(10, 2)		[87004]
	147702.239	(0.040)	2(2, 0) - 1(1, 1)		[87004]
	147808.672	(0.040)	6(2, 4) - 6(1, 5)		[87004]
	148015.665	(0.040)	6(3, 4) - 6(2, 5)		[87004]
	148114.191	(0.040)	4(1, 4) - 3(0, 3)		[87004]
	148744.519	(0.080)	24(18, 6) - 24(17, 7)		[87004]
	148864.058	(0.040)	12(9, 4) - 12(8, 5)		[87004]
	174613.120	(0.040)	18(12, 6) - 18(11, 7)		[87004]
	175201.359	(0.040)	14(10, 5) - 14(9, 6)		[87004]
	175323.639	(0.050)	13(9, 5) - 13(8, 6)		[87004]
	175553.247	(0.040)	16(13, 4) - 16(12, 5)		[87004]
	177297.768	(0.060)	11(7, 5) - 11(6, 6)		[87004]
	177562.283	(0.060)	10(5, 5) - 10(4, 6)		[87004]
	178499.330	(0.030)	10(6, 5) - 10(5, 6)		[87004]
	178585.173	(0.040)	15(13, 3) - 15(12, 4)		[87004]
	178731.439	(0.040)	16(12, 5) - 16(11, 6)		[87004]
	179247.753	(0.060)	9(4, 5) - 9(3, 6)		[87004]
	179576.657	(0.070)	9(5, 5) - 9(4, 6)		[87004]
	179709.946	(1.00)	4(1, 3) - 3(2, 2)		[87004]
	180350.775	(0.030)	8(3, 5) - 8(2, 6)		[87004]
	180448.442	(0.050)	8(4, 5) - 8(3, 6)		[87004]
	180959.762	(0.030)	5(0, 5) - 4(1, 4)		[87004]
	180964.933	(0.030)	5(1, 5) - 4(0, 4)		[87004]
	181076.404	(0.030)	7(2, 5) - 7(1, 6)		[87004]
	181099.574	(0.030)	7(3, 5) - 7(2, 6)		[87004]
	181549.152	(0.030)	6(1, 5) - 6(0, 6)		[87004]
	181553.155	(0.030)	6(2, 5) - 6(1, 6)		[87004]
	183129.932	(0.050)	17(13, 5) - 17(12, 6)		[87004]
	184044.265	(0.030)	14(13, 1) - 14(12, 2)		[87004]
	185055.038	(0.030)	16(14, 2) - 16(13, 3)		[87004]
	185523.086	(0.030)	17(11, 6) - 17(10, 7)		[87004]
	186711.238	(0.040)	14(13, 2) - 14(12, 3)		[87004]

TABLE 9.3. Microwave spectrum of cyclopropenylidene — Continued

C₃H₂

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	$F' - F''$	Ref.
	187145.455	(0.040)	17(14, 4) - 17(13, 5)		[87004]
	194151.163	(0.050)	16(10, 6) - 16(9, 7)		[87004]
	198205.561	(0.050)	19(15, 5) - 19(14, 6)		[87004]
	200320.180	(0.050)	18(15, 4) - 18(14, 5)		[87004]
	200455.279	(0.050)	15(9, 6) - 15(8, 7)		[87004]
	210517.874	(0.030)	12(7, 6) - 12(6, 7)		[87004]
	211148.987	(0.080)	14(14, 0) - 14(13, 1)		[87004]
	211294.440	(0.080)	14(14, 1) - 14(13, 2)		[87004]
	211803.069	(0.030)	11(6, 6) - 11(5, 7)		[87004]
	212457.672	(0.030)	3(3, 0) - 2(2, 1)		[87004]
	212787.837	(0.030)	10(4, 6) - 10(3, 7)		[87004]
	212831.126	(0.030)	10(5, 6) - 10(4, 7)		[87004]
	213024.399	(0.050)	21(16, 6) - 21(15, 7)		[87004]
	213610.032	(0.030)	9(3, 6) - 9(2, 7)		[87004]
	213621.174	(0.060)	9(4, 6) - 9(3, 7)		[87004]
	213872.779	(0.030)	5(1, 4) - 4(2, 3)		[87004]
	214204.883	(0.030)	8(2, 6) - 8(1, 7)		[87004]
	214207.154	(0.030)	8(3, 6) - 8(2, 7)		[87004]
	214289.476	(0.040)	20(13, 7) - 20(12, 8)		[87004]
	214313.034	(0.030)	5(2, 4) - 4(1, 3)		[87004]
	214733.266	(0.030)	19(16, 4) - 19(15, 5)		[87004]
	215640.852	(0.060)	22(18, 4) - 22(17, 5)		[87004]
	218144.439	(0.030)	16(15, 1) - 16(14, 2)		[87004]
	218882.838	(0.030)	16(15, 2) - 16(14, 3)		[87004]
	220443.116	(0.080)	22(17, 6) - 22(16, 7)		[87004]
	221232.367	(0.060)	22(17, 5) - 22(16, 6)		[87004]
	222005.497	(0.060)	20(17, 3) - 20(16, 4)		[87004]
	223160.614	(0.060)	19(12, 7) - 19(11, 8)		[87004]
	224958.482	(0.060)	18(16, 3) - 18(15, 4)		[87004]
	244025.570	(1.20)	13(7, 7) - 13(6, 8)		[87004]
	245141.334	(1.00)	12(5, 7) - 12(4, 8)		[87004]
	245159.726	(1.00)	12(6, 7) - 12(5, 8)		[87004]
	246055.002	(1.20)	11(4, 7) - 11(3, 8)		[87004]
	246723.236	(0.050)	7(1, 7) - 6(0, 6)		[87004]
	246723.236	(0.050)	7(0, 7) - 6(1, 6)		[87004]
	246911.608	(0.050)	6(1, 5) - 5(2, 4)		[87004]
	246958.487	(0.050)	6(2, 5) - 5(1, 4)		[87004]
CDCCH	19418.661	(0.002)	1(1, 0) - 1(0, 1)	1 - 1	[87016]
□	19418.686	(0.002)	1(1, 0) - 1(0, 1)	2 - 1	[87016]
	19418.712	(0.002)	1(1, 0) - 1(0, 1)	1 - 2	[87016]
	19418.724	(0.002)	1(1, 0) - 1(0, 1)	0 - 1	[87016]
	19418.740	(0.002)	1(1, 0) - 1(0, 1)	2 - 2	[87016]
	19418.796	(0.002)	1(1, 0) - 1(0, 1)	1 - 0	[87016]
	118648.117	(0.030)	2(2, 1) - 1(1, 0)		[87004]
	119396.502	(0.030)	11(6, 5) - 11(5, 6)		[87004]
	119721.190	(0.030)	7(5, 3) - 7(4, 4)		[87004]
	121662.307	(0.030)	7(3, 4) - 7(2, 5)		[87004]
	124603.681	(0.030)	15(9, 6) - 15(8, 7)		[87004]
	125236.615	(0.030)	14(9, 5) - 14(8, 6)		[87004]
	128708.888	(0.040)	14(8, 6) - 14(7, 7)		[87004]
	129127.678	(0.030)	7(6, 2) - 7(5, 3)		[87004]
	130139.831	(0.030)	6(2, 4) - 6(1, 5)		[87004]
	132379.889	(0.040)	8(6, 3) - 8(5, 4)		[87004]
	134451.386	(0.030)	7(4, 4) - 7(3, 5)		[87004]
	134461.389	(0.030)	6(3, 4) - 6(2, 5)		[87004]
	134511.003	(0.040)	5(1, 4) - 5(0, 5)		[87004]
	134602.134	(0.080)	10(5, 5) - 10(4, 6)		[87004]
	134898.237	(0.040)	16(10, 6) - 16(9, 7)		[87004]
	135492.872	(0.050)	5(2, 4) - 5(1, 5)		[87004]
	135640.900	(0.030)	4(0, 4) - 3(1, 3)		[87004]
	136370.910	(0.030)	4(1, 4) - 3(0, 3)		[87004]
	136848.255	(0.030)	8(5, 4) - 8(4, 5)		[87004]
	136932.367	(0.030)	11(8, 3) - 11(7, 4)		[87004]
	137454.464	(0.030)	2(2, 0) - 1(1, 1)		[87004]
	140474.074	(0.030)	17(10, 7) - 17(9, 8)		[87004]
	142988.458	(0.030)	9(6, 4) - 9(5, 5)		[87004]
	143041.991	(0.030)	13(7, 6) - 13(6, 7)		[87004]

TABLE 9.3. Microwave spectrum of cyclopropenylidene — Continued

C₃H₂

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	$F' - F''$	Ref.
	143565.383	(0.030)	8(7, 1) - 8(6, 2)		[87004]
	145450.915	(0.030)	13(9, 4) - 13(8, 5)		[87004]
	145505.815	(0.030)	18(11, 7) - 18(10, 8)		[87004]
	148425.563	(0.030)	9(4, 5) - 9(3, 6)		[87004]
	148842.349	(0.030)	3(2, 2) - 2(1, 1)		[87004]
	149331.540	(0.030)	9(7, 3) - 9(6, 4)		[87004]
	149807.503	(0.030)	16(9, 7) - 16(8, 8)		[87004]
	163900.098	(0.030)	7(3, 5) - 7(2, 6)		[87004]
	165432.051	(0.050)	6(1, 5) - 6(0, 6)		[87004]
	165642.855	(0.050)	6(2, 5) - 6(1, 6)		[87004]
	165983.748	(0.030)	11(7, 5) - 11(6, 6)		[87004]
	166112.362	(0.030)	5(0, 5) - 4(1, 4)		[87004]
	166250.124	(0.050)	5(1, 5) - 4(0, 4)		[87004]
	166395.951	(0.030)	19(12, 7) - 19(11, 8)		[87004]
	167904.648	(0.060)	15(8, 7) - 15(7, 8)		[87004]
	168983.683	(0.030)	11(8, 4) - 11(7, 5)		[87004]
	169680.527	(0.030)	10(8, 3) - 10(7, 4)		[87004]
	169821.505	(0.030)	12(9, 3) - 12(8, 4)		[87004]
	170683.853	(0.030)	9(8, 1) - 9(7, 2)		[87004]
	172584.294	(0.030)	18(10, 8) - 18(9, 9)		[87004]
	173586.223	(0.030)	9(8, 2) - 9(7, 3)		[87004]
	173911.588	(0.050)	4(2, 3) - 3(1, 2)		[87004]
	174746.106	(0.040)	12(8, 5) - 12(7, 6)		[87004]
	175315.070	(0.030)	11(5, 6) - 11(4, 7)		[87004]
	179794.241	(0.030)	14(10, 4) - 14(9, 5)		[87004]
	184946.524	(0.030)	10(4, 6) - 10(3, 7)		[87004]
	186357.734	(0.030)	12(7, 6) - 12(6, 7)		[87004]
	186860.305	(0.040)	11(9, 2) - 11(8, 3)		[87004]
	186919.958	(0.030)	11(6, 6) - 11(5, 7)		[87004]
	187183.625	(0.030)	14(7, 7) - 14(6, 8)		[87004]
	187926.732	(0.030)	16(11, 5) - 16(10, 6)		[87004]
	193782.524	(0.030)	17(9, 8) - 17(8, 9)		[87004]
	193930.163	(0.030)	8(2, 6) - 8(1, 7)		[87004]
	194196.258	(0.040)	8(3, 6) - 8(2, 7)		[87004]
	194367.304	(0.030)	5(1, 4) - 4(2, 3)		[87004]
	194510.019	(0.030)	18(12, 6) - 18(11, 7)		[87004]
	195733.056	(0.030)	14(9, 6) - 14(8, 7)		[87004]
	195973.432	(0.040)	7(1, 6) - 7(0, 7)		[87004]
	196014.148	(0.050)	7(2, 6) - 7(1, 7)		[87004]
	196354.879	(0.030)	6(0, 6) - 5(1, 5)		[87004]
	196378.448	(0.030)	6(1, 6) - 5(0, 5)		[87004]
	196408.150	(0.030)	10(9, 1) - 10(8, 2)		[87004]
	196911.530	(0.030)	20(11, 9) - 20(10, 10)		[87004]
	199319.827	(0.030)	5(2, 4) - 4(1, 3)		[87004]
	199915.622	(0.030)	20(13, 7) - 20(12, 8)		[87004]
	200294.630	(0.030)	3(3, 0) - 2(2, 1)		[87004]
	201139.060	(0.030)	13(10, 3) - 13(9, 4)		[87004]
	202258.579	(0.030)	13(6, 7) - 13(5, 8)		[87004]
	203812.890	(0.030)	5(2, 3) - 4(3, 2)		[87004]
	206200.330	(0.030)	14(10, 5) - 14(9, 6)		[87004]
	207475.381	(0.030)	15(10, 6) - 15(9, 7)		[87004]
	210950.643	(0.030)	14(8, 7) - 14(7, 8)		[87004]
	211828.536	(0.030)	15(9, 7) - 15(8, 8)		[87004]
	212105.543	(0.030)	12(5, 7) - 12(4, 8)		[87004]
	212803.902	(0.030)	13(7, 7) - 13(6, 8)		[87004]
	213491.394	(0.050)	15(11, 4) - 15(10, 5)		[87004]
	213872.297	(1.00)	12(10, 2) - 12(9, 3)		[87004]
	214070.086	(0.030)	16(8, 8) - 16(7, 9)		[87004]
	216092.555	(0.040)	12(10, 3) - 12(9, 4)		[87004]
	216779.279	(0.030)	16(10, 7) - 16(9, 8)		[87004]
	218181.896	(0.030)	11(4, 7) - 11(3, 8)		[87004]
	219356.349	(0.030)	11(5, 7) - 11(4, 8)		[87004]
	220438.926	(0.030)	19(10, 9) - 19(9, 10)		[87004]
	221375.758	(0.030)	11(10, 1) - 11(9, 2)		[87004]
	221697.066	(0.030)	4(3, 2) - 3(2, 1)		[87004]
	221767.949	(0.030)	11(10, 2) - 11(9, 3)		[87004]
	222042.345	(0.030)	10(3, 7) - 10(2, 8)		[87004]

TABLE 9.3. Microwave spectrum of cyclopropenylidene — Continued

C₃H₂

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	$F' - F''$	Ref.
	223905.102	(0.030)	17(12, 5)	- 17(11, 6)	[87004]
	223910.842	(0.030)	16(11, 6)	- 16(10, 7)	[87004]
	224625.290	(0.030)	9(2, 7)	- 9(1, 8)	[87004]
	224680.568	(0.030)	9(3, 7)	- 9(2, 8)	[87004]
	226294.111	(0.030)	6(1, 5)	- 5(2, 4)	[87004]
	226553.556	(0.050)	7(0, 7)	- 6(1, 6)	[87004]
	226557.218	(0.050)	7(1, 7)	- 6(0, 6)	[87004]
	227510.300	(0.030)	6(2, 5)	- 5(1, 4)	[87004]
	240445.135	(0.050)	13(11, 3)	- 13(10, 4)	[87004]
	244165.350	(0.030)	17(12, 6)	- 17(11, 7)	[87004]
	244249.938	(0.030)	16(12, 4)	- 16(11, 5)	[87004]
	245521.528	(0.030)	13(5, 8)	- 13(4, 9)	[87004]
	246616.267	(0.030)	13(6, 8)	- 13(5, 9)	[87004]
	248914.222	(0.030)	6(2, 4)	- 5(3, 3)	[87004]
	249841.456	(0.030)	12(4, 8)	- 12(3, 9)	[87004]
	250132.496	(0.030)	12(5, 8)	- 12(4, 9)	[87004]
	250740.604	(0.030)	16(12, 5)	- 16(11, 6)	[87004]
	280885.777	(0.030)	13(4, 9)	- 13(3,10)	[87004]
	280951.936	(0.030)	13(5, 9)	- 13(4,10)	[87004]
	283560.936	(1.00)	12(3, 9)	- 12(2,10)	[87004]
	283574.008	(1.00)	12(4, 9)	- 12(3,10)	[87004]
	284905.753	(0.080)	20(11,10)	- 20(10,11)	[87004]
	285163.964	(0.030)	7(2, 5)	- 6(3, 4)	[87004]
	286923.752	(0.030)	19(14, 5)	- 19(13, 6)	[87004]
	286933.385	(0.050)	9(0, 9)	- 8(1, 8)	[87004]
	286933.385	(0.050)	9(1, 9)	- 8(0, 8)	[87004]
	287136.993	(0.030)	8(1, 7)	- 7(2, 6)	[87004]
	287185.594	(0.030)	8(2, 7)	- 7(1, 6)	[87004]
	289933.402	(0.040)	19(10,10)	- 19(9,11)	[87004]
	290899.576	(0.030)	7(3, 5)	- 6(2, 4)	[87004]
	292728.746	(0.030)	18(8,10)	- 18(7,11)	[87004]
	295213.145	(0.040)	7(3, 4)	- 6(4, 3)	[87004]
	295377.145	(0.050)	18(9,10)	- 18(8,11)	[87004]
	296782.707	(0.050)	5(4, 2)	- 4(3, 1)	[87004]

Table 10.1. Molecular constants for allene in vibrationally excited states. [87017]

Parameter	Vibrational State		
	$v_{11} = 1$	$v_{10} = 1$	$v_9 = 1$
B (MHz)	8904.434(4)	8879.325(7)	8890.310(20)
D_J (kHz)	3.58(63)	3.50(83)	2.65 ^a
μ (D)	0.010(1)	0.0452(6)	

^aValue fixed.Table 10.2 Molecular constants for allene-d₁ and allene-1,1-d₂. [86012]

Parameter	Vibrational State	
	CDHCCH ₂	CD ₂ CCH ₂
A (MHz)	117600.541(744)	96431.962 ^a
B (MHz)	8374.299(39)	7955.141(7)
C (MHz)	8261.946(41)	7737.167(7)
Δ_J (kHz)	3.06(44)	2.374(270)
Δ_{JK} (kHz)	154.(19)	129.57(84)
Δ_K (kHz)	2160.(460)	1316. ^a
δ_J (kHz)	0.0635(12)	0.0758(4)
δ_K (kHz)	-87.2(25)	-2.24(19)

Electric Dipole Moment [73081]

μ (D)	0.0031(3)
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^aConstrained at the value from F. Hegelund and J. Kauppinen, J. Mol. Spectrosc. **110** 106 (1985).

TABLE 10.3. Microwave spectrum of allene

C₃H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
H ₂ CCCH ₂	17758.637	(0.005)	1(0, 1) - 0(0, 0)	1ν ₁₀	[87017]
	17780.610	(0.018)	1(0, 1) - 0(0, 0)	1ν ₉	[87017]
	17808.853	(0.001)	1(0, 1) - 0(0, 0)	1ν ₁₁	[87017]
	35517.190	(0.010)	2(0, 2) - 1(0, 1)	1ν ₁₀	[87017]
	35617.620	(0.010)	2(0, 2) - 1(0, 1)	1ν ₁₁	[87017]
D ₂ CCCH ₂	7846.450	(0.050)	8(1, 7) - 8(1, 8)		[86012]
	8066.768	(0.050)	26(2,24) - 26(2,25)		[86012]
	9327.856	(0.050)	27(2,25) - 27(2,26)		[86012]
	9807.638	(0.050)	9(1, 8) - 9(1, 9)		[86012]
	10725.376	(0.050)	28(2,26) - 28(2,27)		[86012]
	11986.452	(0.050)	10(1, 9) - 10(1,10)		[86012]
	12267.147	(0.050)	29(2,27) - 29(2,28)		[86012]
	13960.898	(0.050)	30(2,28) - 30(2,29)		[86012]
	14382.877	(0.050)	11(1,10) - 11(1,11)		[86012]
	15692.292	(0.050)	1(0, 1) - 0(0, 0)		[86012]
	15814.124	(0.050)	31(2,29) - 31(2,30)		[86012]
	16996.737	(0.050)	12(1,11) - 12(1,12)		[86012]
	17834.190	(0.050)	32(2,30) - 32(2,31)		[86012]
	47073.55	(0.10)	3(2, 2) - 2(2, 1)		[73081]
	47075.18	(0.10)	3(2, 1) - 2(2, 0)		[73081]
	62760.10	(0.10)	4(3, 2) - 3(3, 1)		[73081]
	62760.10	(0.10)	4(3, 1) - 3(3, 0)		[73081]
	62764.18	(0.10)	4(2, 3) - 3(2, 2)		[73081]
	62768.17	(0.10)	4(2, 2) - 3(2, 1)		[73081]
	DHCCCH ₂	7436.207	(0.050)	19(2,17) - 20(1,20)	
7892.260		(0.050)	21(1,21) - 20(2,18)		[86012]
8349.456		(0.050)	7(0, 7) - 6(1, 6)		[86012]
8620.983		(0.050)	5(1, 5) - 6(0, 6)		[86012]
8787.459		(0.050)	12(1,11) - 12(1,12)		[86012]
10251.262		(0.050)	13(1,12) - 13(1,13)		[86012]
10669.538		(0.050)	32(2,30) - 31(3,29)		[86012]
11827.560		(0.050)	14(1,13) - 14(1,14)		[86012]
13516.132		(0.050)	15(1,14) - 15(1,15)		[86012]
14749.380		(0.050)	31(3,28) - 32(2,31)		[86012]
15316.867		(0.050)	16(1,15) - 16(1,16)		[86012]
16636.279		(0.050)	1(0, 1) - 0(0, 0)		[86012]
16728.297		(0.050)	20(1,19) - 19(2,18)		[86012]
18218.606		(0.050)	34(2,33) - 33(3,30)		[86012]
18720.821		(0.050)	17(2,16) - 18(1,17)		[86012]

Table 11.1. Molecular constants for cyclopropene and 1,2-dideuterocyclopropene.

Parameter	$\begin{array}{c} \text{CH}_2 \\ / \quad \backslash \\ \text{HC}=\text{CH} \end{array}$		$\begin{array}{c} \text{CH}_2 \\ / \quad \backslash \\ \text{DC}=\text{CD} \end{array}$	
A'' (MHz)	30061.2906(16)		23178.165(25)	
B'' (MHz)	21825.7814(10)		20102.070(25)	
C'' (MHz)	13795.7624(8)		11585.453(17)	
τ_1 (MHz)	-0.486516(89)		-0.2772(426)	
τ_2 (MHz)	-0.121949(28)		-0.0667(136)	
τ_3 (MHz)	4.1633(4)		5.1(2)	
τ_{aaaa} (MHz)	-0.207119(78)		-0.1357(57)	
τ_{bbbb} (MHz)	-0.154729(22)		-0.1389(109)	
τ_{cccc} (MHz)	-0.026625(18)		----	
H _{JK} (Hz)	-0.393(96)			
H _{KJ} (Hz)	1.69(29)			
H _K (Hz)	-1.354(380)			
h _J (Hz)	0.0364(12)			
h _{JK} (Hz)	-0.168(54)			
h _K (Hz)	1.249(13)			
<u>Dipole moment</u> [59017]				
μ_a (D)	0.454(10)		0.461(10)	

Table 11.2. Molecular constants for $^{13}\text{C}_1$, $^{13}\text{C}_2$, D₂ (methylene) and D (ethylenic) species of cyclopropene.

Parameter [Reference]	$\begin{array}{c} \text{CH}_2 \\ / \quad \backslash \\ \text{HC}=\text{CH} \end{array}$ [75050]	$\begin{array}{c} ^{13}\text{CH}_2 \\ / \quad \backslash \\ \text{HC}=\text{CH} \end{array}$ [75050]	$\begin{array}{c} \text{HCD} \\ / \quad \backslash \\ \text{HC}=\text{CH} \end{array}$ [75050]	$\begin{array}{c} \text{CH}_2 \\ / \quad \backslash \\ \text{DC}=\text{CH} \end{array}$ [59017]
	A (MHz)	30062.00(31)	29369.26(24)	28792.96(21)
B (MHz)	21129.22(22)	21601.94(18)	19356.66(19)	20520.1
C (MHz)	13513.62(22)	13560.06(18)	13011.74(19)	12606.1
<u>Dipole moments</u> [59017]				
μ_a (D)			0.446	0.443
μ_b (D)			0	0.156(20)
μ_c (D)			0.443	0

TABLE 11.3. Microwave spectrum of cyclopropene

C₃H₄


Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$	$- J''(K_{-1}, K_{+1})$	Ref.
CHCH ₂ CH 	15089.620	(0.030)	3(2, 1)	- 3(2, 2)	[69055]
	19247.250	(0.020)	29(16,13)	- 29(16,14)	[75050]
	19784.260	(0.020)	12(7, 5)	- 12(7, 6)	[75050]
CH=CH \ / CH ₂	20488.440	(0.020)	31(17,14)	- 31(17,15)	[75050]
	21544.196	(0.030)	5(3, 2)	- 5(3, 3)	[69055]
	21699.560	(0.020)	33(18,15)	- 33(18,16)	[75050]
	22728.940	(0.020)	14(8, 6)	- 14(8, 7)	[75050]
	22880.100	(0.020)	35(19,16)	- 35(19,17)	[75050]
	24029.680	(0.020)	37(20,17)	- 37(20,18)	[75050]
	24089.592	(0.020)	2(1, 1)	- 2(1, 2)	[69055]
	25148.040	(0.020)	39(21,18)	- 39(21,19)	[75050]
	25593.960	(0.020)	16(9, 7)	- 16(9, 8)	[75050]
	27599.740	(0.020)	7(4, 3)	- 7(4, 4)	[75050]
	28382.210	(0.020)	18(10, 8)	- 18(10, 9)	[75050]
	31095.940	(0.020)	20(11, 9)	- 20(11,10)	[75050]
	33353.410	(0.020)	9(5, 4)	- 9(5, 5)	[75050]
	33737.110	(0.020)	22(12,10)	- 22(12,11)	[75050]
	34935.353	(0.020)	4(2, 2)	- 4(2, 3)	[69055]
	35621.290	(0.020)	1(0, 1)	- 0(0, 0)	[69055]
	36306.970	(0.020)	24(13,11)	- 24(13,12)	[75050]
	38807.120	(0.020)	26(14,12)	- 26(14,13)	[75050]
	38860.280	(0.020)	11(6, 5)	- 11(6, 6)	[75050]
	39098.420	(0.020)	3(0, 3)	- 2(2, 0)	[75050]
	92868.180	(0.010)	3(1, 3)	- 2(1, 2)	[87008]
	95444.193	(0.010)	3(0, 3)	- 2(0, 2)	[87008]
	98817.024	(0.010)	5(1, 4)	- 5(1, 5)	[87008]
	101782.053	(0.010)	5(2, 4)	- 5(0, 5)	[87008]
	102488.675	(0.010)	6(3, 4)	- 6(1, 5)	[87008]
	106860.325	(0.010)	3(2, 2)	- 2(2, 1)	[87008]
	108505.921	(0.010)	12(4, 9)	- 11(6, 6)	[87008]
	128959.020	(0.020)	28(14,14)	- 28(14,15)	[86006]
	130207.269	(0.020)	9(5, 5)	- 9(3, 6)	[86006]
	130719.509	(0.030)	11(5, 7)	- 10(7, 4)	[86006]
	131660.858	(0.020)	17(8, 9)	- 17(8,10)	[86006]
	134337.198	(0.030)	15(9, 7)	- 14(11, 4)	[86006]
	135126.122	(0.020)	7(5, 3)	- 7(3, 4)	[86006]
	135147.198	(0.020)	9(3, 6)	- 9(3, 7)	[86006]
	135227.870	(0.020)	30(15,15)	- 30(15,16)	[86006]
	135485.125	(0.020)	12(5, 7)	- 12(5, 8)	[86006]
135786.145	(0.030)	16(4,12)	- 15(6, 9)	[86006]	
149279.120	(0.010)	5(1, 5)	- 4(1, 4)	[87008]	
149432.519	(0.010)	14(6, 8)	- 14(6, 9)	[87008]	
149548.939	(0.010)	5(0, 5)	- 4(0, 4)	[87008]	
152662.769	(0.010)	19(5,14)	- 18(7,11)	[87008]	
161402.303	(0.020)	10(3, 7)	- 10(3, 8)	[86006]	
161478.222	(0.020)	23(11,12)	- 23(11,13)	[86006]	
161958.377	(0.020)	12(6, 7)	- 12(4, 8)	[86006]	
162920.429	(0.020)	16(7, 9)	- 16(7,10)	[86006]	
163010.373	(0.010)	18(11, 8)	- 17(13, 5)	[87008]	
163820.198	(0.020)	10(4, 7)	- 10(2, 8)	[86006]	
164054.815	(0.030)	40(20,20)	- 40(20,21)	[86006]	
165360.735	(0.010)	14(8, 6)	- 13(10, 3)	[87008]	
166147.003	(0.010)	10(5, 5)	- 9(7, 2)	[87008]	
166421.837	(0.020)	9(2, 7)	- 9(2, 8)	[86006]	
166901.060	(0.020)	9(3, 7)	- 9(1, 8)	[86006]	
168570.295	(0.020)	13(5, 8)	- 13(5, 9)	[86006]	
169401.329	(0.020)	8(1, 7)	- 8(1, 8)	[86006]	
169445.995	(0.020)	8(3, 5)	- 7(5, 2)	[86006]	
169465.977	(0.020)	8(2, 7)	- 8(0, 8)	[86006]	
170089.110	(0.020)	5(2, 4)	- 4(2, 3)	[86006]	
170863.101	(0.020)	25(12,13)	- 25(12,14)	[86006]	
170932.920	(0.010)	13(7, 7)	- 13(5, 8)	[87008]	
171570.082	(0.020)	5(4, 1)	- 5(2, 4)	[86006]	
171862.920	(0.020)	13(6, 8)	- 12(8, 5)	[86006]	
172700.264	(0.010)	12(7, 6)	- 12(5, 8)	[87008]	
174623.476	(0.020)	3(2, 1)	- 2(0, 2)	[86006]	
174915.602	(0.010)	5(1, 4)	- 4(1, 3)	[87008]	
176000.634	(0.020)	18(8,10)	- 18(8,11)	[86006]	

TABLE 11.3. Microwave spectrum of cyclopropene — Continued

C₃H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
	176563.929	(0.020)	9(4, 5) - 8(6, 2)	[86006]
	176954.339	(0.020)	6(1, 6) - 5(1, 5)	[86006]
	177022.433	(0.010)	6(0, 6) - 5(0, 5)	[87008]
	180569.324	(0.010)	8(6, 3) - 8(4, 4)	[87008]
	184626.564	(0.020)	14(7, 8) - 13(9, 5)	[87008]
	190269.093	(0.010)	25(8,18) - 24(10,15)	[87008]
	193665.941	(0.020)	9(3, 6) - 8(5, 3)	[86006]
	194658.487	(0.020)	14(8, 7) - 14(6, 8)	[86006]
	195615.548	(0.020)	6(5, 1) - 6(3, 4)	[86006]
	195955.301	(0.020)	3(3, 0) - 2(1, 1)	[86006]
	196379.160	(0.020)	21(6,15) - 20(8,12)	[87008]
	196397.198	(0.010)	5(2, 3) - 4(2, 2)	[87008]
	197254.017	(0.020)	14(5, 9) - 15(5,10)	[86006]
	197495.388	(0.020)	5(3, 2) - 4(3, 1)	[86006]
	197570.049	(0.010)	31(15,16) - 31(15,17)	[87008]
	198316.905	(0.020)	15(7, 9) - 15(5,10)	[86006]
	199136.982	(0.020)	6(2, 5) - 5(2, 4)	[87008]
	199301.345	(0.020)	16(8, 9) - 16(6,10)	[86006]
	199905.686	(0.020)	17(7,10) - 17(7,11)	[86006]
	201087.180	(0.020)	22(10,12) - 22(10,13)	[86006]
	201120.278	(0.020)	6(1, 5) - 5(1, 4)	[86006]
	201272.394	(0.010)	7(6, 2) - 7(4, 3)	[87008]
	201560.781	(0.020)	14(6, 9) - 14(4,10)	[86006]
	204121.257	(0.020)	6(4, 2) - 6(2, 5)	[86006]
	204560.676	(0.020)	7(1, 6) - 6(1, 6)	[86006]
	204576.617	(0.020)	7(0, 7) - 6(0, 6)	[86006]
	204732.293	(0.010)	13(4, 9) - 13(4,10)	[87008]
	205826.400	(0.020)	13(5, 9) - 13(3,10)	[86006]
	206024.480	(0.020)	33(16,17) - 33(16,18)	[86006]
	258536.982	(0.020)	20(11,10) - 20(9,11)	[86006]
	258613.762	(0.020)	19(7,12) - 19(7,13)	[86006]
	258619.637	(0.050)	32(15,17) - 32(15,18)	[86006]
	258797.927	(0.020)	13(2,11) - 13(2,12)	[86006]
	259733.320	(0.200)	9(0, 9) - 8(0, 8)	[86006]
	259733.320	(0.200)	9(1, 9) - 8(1, 8)	[86006]
	260042.732	(0.020)	7(4, 4) - 6(4, 3)	[86006]
	260780.767	(0.020)	7(6, 1) - 6(6, 0)	[86006]
	260963.843	(0.020)	19(8,12) - 19(6,13)	[86006]
	261021.910	(0.200)	12(2,11) - 12(0,12)	[86006]
	261021.910	(0.200)	12(1,11) - 12(1,12)	[86006]
	261051.753	(0.020)	17(10, 8) - 17(8, 9)	[86006]
	262442.820	(0.020)	7(5, 3) - 6(5, 2)	[86006]
	263535.563	(0.020)	22(9,13) - 22(9,14)	[86006]
	265663.338	(0.020)	7(5, 2) - 6(5, 1)	[86006]
	266019.889	(0.020)	18(6,12) - 18(6,13)	[86006]
	266640.816	(0.020)	18(7,12) - 18(5,13)	[86006]
	266861.064	(0.020)	23(12,12) - 23(10,13)	[86006]
	267176.301	(0.020)	14(9, 6) - 14(7, 7)	[86006]
	268385.389	(0.020)	23(11,13) - 23(9,14)	[86006]
	270473.476	(0.020)	24(12,13) - 24(10,14)	[86006]
	271446.951	(0.020)	17(5,12) - 17(5,13)	[86006]
	271587.728	(0.020)	17(6,12) - 17(4,13)	[86006]
	271631.600	(0.070)	27(12,15) - 27(12,16)	[86006]
	272482.493	(0.020)	22(10,13) - 22(8,14)	[86006]
	274950.092	(0.040)	10(7, 3) - 10(5, 6)	[86006]
	275664.418	(0.020)	16(4,12) - 16(4,13)	[86006]
	275691.261	(0.020)	16(5,12) - 16(3,13)	[86006]
	275802.194	(0.020)	21(8,13) - 21(8,14)	[86006]
	276292.091	(0.020)	12(5, 7) - 11(7, 4)	[86006]
	277108.711	(0.020)	8(3, 6) - 7(3, 5)	[86006]
	277212.986	(0.020)	7(4, 3) - 6(4, 2)	[86006]
	277312.300	(0.020)	7(3, 4) - 6(3, 3)	[86006]
	325642.564	(0.020)	9(4, 6) - 8(4, 5)	[86006]
	332580.788	(0.040)	22(7,15) - 22(7,16)	[86006]
	333187.194	(0.020)	10(3, 8) - 9(3, 7)	[86006]
	333522.130	(0.020)	10(2, 8) - 9(2, 7)	[86006]
	334362.950	(0.020)	9(8, 2) - 8(8, 1)	[86006]

TABLE 11.3. Microwave spectrum of cyclopropene — Continued

C₃H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
	334645.654	(0.020)	9(3, 6) - 8(3, 5)	[86006]
	336811.212	(0.020)	9(7, 3) - 8(7, 2)	[86006]
	337131.062	(0.020)	9(7, 2) - 8(7, 1)	[86006]
	337500.944	(0.020)	21(7, 15) - 21(5, 16)	[86006]
	337513.419	(0.020)	9(5, 5) - 8(5, 4)	[86006]
	337779.745	(0.020)	11(2, 10) - 10(2, 9)	[86006]
	337782.580	(0.020)	11(1, 10) - 10(1, 9)	[86006]
	339348.140	(0.020)	9(6, 4) - 8(6, 3)	[86006]
	342473.856	(0.050)	12(1, 12) - 11(1, 11)	[86006]
	342473.856	(0.050)	12(0, 12) - 11(0, 11)	[86006]
	343502.309	(0.020)	9(6, 3) - 8(6, 2)	[86006]
	388329.470	(0.020)	12(3, 10) - 11(3, 9)	[86006]
	388354.773	(0.020)	12(2, 10) - 11(2, 9)	[86006]
	389373.044	(0.020)	10(4, 6) - 9(4, 5)	[86006]
	389488.619	(0.020)	10(6, 4) - 9(6, 3)	[86006]
	392915.652	(0.200)	13(1, 12) - 12(1, 11)	[86006]
	392915.652	(0.200)	13(2, 12) - 12(2, 11)	[86006]
	397625.816	(0.050)	14(0, 14) - 13(0, 13)	[86006]
	397625.816	(0.050)	14(1, 14) - 13(1, 13)	[86006]
	401513.206	(0.020)	10(5, 5) - 9(5, 4)	[86006]
	403820.287	(0.020)	11(5, 7) - 10(5, 6)	[86006]
	411462.546	(0.020)	12(4, 9) - 11(4, 8)	[86006]
	411976.242	(0.020)	12(3, 9) - 11(3, 8)	[86006]
	413450.659	(0.050)	11(8, 4) - 10(8, 3)	[86006]
	413916.720	(0.050)	11(8, 3) - 10(8, 2)	[86006]
	415328.566	(0.020)	11(6, 6) - 10(6, 5)	[86006]
	452768.740	(0.040)	16(1, 16) - 15(1, 15)	[86006]
	452768.740	(0.040)	16(0, 16) - 15(0, 15)	[86006]
	462079.285	(0.080)	13(5, 9) - 12(5, 8)	[86006]
	470335.604	(0.040)	12(5, 7) - 11(5, 6)	[86006]
	470954.721	(0.200)	15(2, 13) - 14(2, 12)	[86006]
	470954.721	(0.200)	15(3, 13) - 14(3, 12)	[86006]
	475612.842	(0.050)	16(1, 15) - 15(1, 14)	[86006]
	475612.842	(0.050)	16(2, 15) - 15(2, 14)	[86006]
	480336.475	(0.050)	17(1, 17) - 16(1, 16)	[86006]
	480336.475	(0.050)	17(0, 17) - 16(0, 16)	[86006]
	480336.475	(0.050)	17(1, 17) - 16(1, 16)	[86006]
	482190.737	(0.050)	13(6, 8) - 12(6, 7)	[86006]
	482555.735	(0.040)	12(6, 6) - 11(6, 5)	[86006]
¹³ CHCH ₂ CH	19342.29	(0.05)	10(6, 4) - 10(6, 5)	[75050]
	22602.59	(0.05)	5(3, 2) - 5(3, 3)	[75050]
	24125.30	(0.05)	2(1, 1) - 2(1, 2)	[75050]
	29564.40	(0.05)	7(4, 3) - 7(4, 4)	[75050]
	35161.58	(0.05)	1(0, 1) - 0(0, 0)	[75050]
	35547.49	(0.05)	4(2, 2) - 4(2, 3)	[75050]
	36447.37	(0.05)	9(5, 4) - 9(5, 5)	[75050]
CH ¹³ CH ₂ CH	18232.84	(0.05)	5(3, 2) - 5(3, 3)	[75050]
	22134.49	(0.05)	7(4, 3) - 7(4, 4)	[75050]
	22845.80	(0.05)	2(1, 1) - 2(1, 2)	[75050]
	25361.12	(0.05)	9(5, 4) - 9(5, 5)	[75050]
	31859.21	(0.05)	4(2, 2) - 4(2, 3)	[75050]
	34642.43	(0.05)	1(0, 1) - 0(0, 0)	[75050]
	39332.42	(0.10)	6(3, 3) - 6(3, 4)	[75050]
CDCH ₂ CH	20700.90	(0.10)	8(5, 3) - 8(5, 4)	[59017]
	23741.60	(0.10)	2(1, 1) - 2(1, 2)	[59017]
	25209.60	(0.10)	5(3, 2) - 5(3, 3)	[59017]
	27649.20	(0.10)	10(6, 4) - 10(6, 5)	[59017]
	33126.10	(0.10)	1(0, 1) - 0(0, 0)	[59017]
	34726.60	(0.10)	7(4, 3) - 7(4, 4)	[59017]
	35306.10	(0.10)	12(7, 5) - 12(7, 6)	[59017]
	36498.70	(0.10)	4(2, 2) - 4(2, 3)	[59017]
CHCHDCH	19034.30	(0.10)	2(1, 1) - 2(1, 2)	[59017]
	24449.10	(0.10)	4(2, 2) - 4(2, 3)	[59017]
	27632.70	(0.10)	6(3, 3) - 6(3, 4)	[59017]
	28790.10	(0.10)	12(6, 6) - 12(6, 7)	[59017]
	29165.30	(0.10)	8(4, 4) - 8(4, 5)	[59017]
	29446.20	(0.10)	10(5, 5) - 10(5, 6)	[59017]

TABLE 11.3. Microwave spectrum of cyclopropene — Continued

C₃H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J''(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
CDCH ₂ CD □	32368.00	(0.10)	1(0, 1) - 0(0, 0)	[59017]
	37508.90	(0.10)	3(1, 2) - 3(1, 3)	[59017]
	16449.774	(0.030)	4(3, 1) - 4(3, 2)	[69055]
	19647.90	(0.10)	11(8, 3) - 11(8, 4)	[59017]
	21429.055	(0.030)	3(2, 1) - 3(2, 2)	[69055]
	23124.00	(0.10)	7(5, 2) - 7(5, 3)	[59017]
	25549.330	(0.020)	2(1, 1) - 2(1, 2)	[69055]
	28955.50	(0.10)	10(7, 3) - 10(7, 4)	[59017]
	30819.70	(0.10)	6(4, 2) - 6(4, 3)	[59017]
	31687.35	(0.03)	1(0, 1) - 0(0, 0)	[69055]
	35471.348	(0.020)	2(2, 1) - 2(0, 2)	[69055]
	37894.22	(0.02)	5(3, 2) - 5(3, 3)	[69055]

Table 12.1. Molecular constants for propyne and ^{13}C -propyne in the ground vibrational state.

Parameter	CH_3CCH	$^{13}\text{CH}_3\text{CCH}$	$\text{CH}_3\text{-}^{13}\text{CCH}$	$\text{CH}_3\text{C-}^{13}\text{CH}$
<u>Rotational constants</u> [79038]				
B_0 (MHz)	8545.87712(6)	8313.2469(22)	8542.3321(17)	8290.2498(16)
D_J (kHz)	2.9423(7)	2.796(23)	2.936(17)	2.801(16)
D_{JK} (kHz)	163.473(10)	155.201(61)	162.857(59)	155.533(57)
D_K^a (kHz)	2983.	2991.	2984.	2991.
H_{JJJ} (Hz)	0.0097(20)	-0.044(62)	-0.048(50)	0.117(45)
H_{JJK} (Hz)	0.935(68)	0.84(20)	1.24(21)	0.78(18)
H_{JKK} (Hz)	5.23(14)	5.09(67)	4.80(38)	5.56(57)
<u>Dipole moment</u> [66042]				
μ (D)	0.7804			
<u>Magnetic constants</u>				
g_{\perp}	0.00350(15)		[69064]	
g_{\parallel}	0.295		[75055]	
$\chi_{\perp-\chi_{\parallel}}$	$7.74(14)\times 10^{-6}$	erg/G ² ·mol	[69064]	
θ_{\parallel}	$4.82(23)\times 10^{-26}$	esu·cm ²	[69064]	

^aCalculated from the force field in reference [76058].

Table 12.2. Molecular constants for deuterated species of CH_3CCH .^a

Species	B_0	C_0	D_J	D_{JK}	eqQ(D)	Reference
CH_3CCD	7788.1699(26)	---	0.00287(38)	0.1414(25)	0.228(2) ^b	[present]
CD_3CCH	7355.7680(122)	---	0.00227(40)	0.10386(26) ^c	b	[present]
CD_3CCD	6734.32(5)	---	~0.002	0.09		[55018]
CH_2DCCH	8155.67(10)	8025.46(10)	~0.003	0.13		[55018]
CHD_2CCH	7765.73(10)	7630.99(10)	~0.002	0.13		[55018]
CH_2DCCD	7440.77(10)	7331.96(10)	~0.001	0.12		[55018]
CHD_2CCD	7095.09(10)	6982.56(10)	---	0.11		[55018]

Dipole moment for CD_3CCH [70029]

μ (K=0) = 0.78780(13) D

μ (K=2) = 0.78765(21) D

μ (K=3) = 0.78741(14) D

^aRotational, centrifugal distortion and hyperfine constants in MHz.

^bFrom reference [82035]. For CD_3CCH $eq_{aa}Q = -0.0550(5)$ MHz, $eq_{zz}Q = 0.174(6)$ MHz and $c_D = 0.06(9)$ kHz.

^cFrom reference [70029].

Table 12.3. Molecular constants for propyne in the $v_9=1$ and $v_5=1$ vibrational states.

Parameter	$v_9=1$ Excited State	$v_9=2$ Excited State	$v_5=1$ Excited State
<u>Rotational Constants</u>			
A_V (MHz)	142433.	137392.	
B_V (MHz)	8551.0547	8556.1996	8508.119(3)
D_J (MHz)	0.00286	0.00296	0.0018(2)
D_{JK} (MHz)	0.1659	0.1672	0.169(1)
q_V (MHz)	2.2592	2.2613	
q_{12} (MHz)	-5.	-10.	
$ u $ (MHz)	0.00043	---	
ζ_9 (MHz)	1.000	0.94	
$(B_V - C_V + C_V \zeta_9)^{-1}$ (MHz)	0.0001174	---	
η_J (MHz)	0.4645	0.4687	
<u>Electric Dipole Moment</u>			
μ	0.58(12) ^a D		0.7954(10) D
Reference	[86019]	[86019]	[80038]

^aFrom measurement of linewidth.Table 12.4. Molecular constants for propyne in the v_{10} excited state.

Parameter ^a	$v_{10}=1$	$v_{10}=2$	$v_{10}=3$	$v_{10}=4$
B_V^b (MHz)	8569.9919	8593.9546	8617.624	8640.569
D_J (MHz)	0.003018	0.00312	0.0086	0.002974
D_{JK} (MHz)	0.1638	0.1642	0.1095	0.1653
ρ^* (MHz)	0.001950	---	---	---
q_J (MHz)	4.1938	4.1938	4.1778	4.17786
$q_5^2 / (B_V - C_V + \zeta_{10})$ (MHz)	-0.002051	---	---	---
$\gamma_{\ell\ell}$ (MHz)		-0.2164	-0.2143	-0.1798
ζ (MHz)		0.889	0.750	0.76
q_{12} (MHz)		-33.681	-37.64	-38.
d_{12} (MHz)		112.11	77.1	81.
$\chi_{\ell\ell}$ (MHz)		147834.		144800.
η_J (MHz)			0.4007	0.33714
η_{JJ} (MHz)			0.00149	0.00125
η_{JK} (MHz)			0.00296	0.003
α_{10}^b (MHz)		-24.280		
γ_{10}^b (MHz)		0.123		
Reference	[69063]	[85015]	[86007]	[86020]

^aSee references cited for definition of the parameters.^bUncertainties are a few units in the least significant figure. $B_{V_{10}} = B_0 - \alpha_{10} - q_{10} + \gamma_{11}$ and $B_{2V_{10}} = B_0 - 2\alpha_{10} - 4\gamma_{10}$.

TABLE 12.5. Microwave spectrum of propyne

C₃H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' K'$	-	$J'' K''$	$F' F'_1$	-	$F'' F''_1$	Vib. state	Ref.
CH ₃ CCH	17016.231	(0.010)	1(0)	-	0(0)				1ν ₅	[80038]
	17091.718	(0.030)	1(0)	-	0(0)					[84032]
	17102.050	(0.050)	1(0)	-	0(0)				1ν ₉ ℓ = +1	[84032]
	17139.588	(0.050)	1(0)	-	0(0)				1ν ₁₀ ℓ = +1	[84032]
	17186.451	(0.100)	1(0)	-	0(0)				2ν ₁₀ ℓ = +2	[85015]
	17187.337	(0.100)	1(0)	-	0(0)				2ν ₁₀ ℓ = +0	[85015]
	17232.13	(0.10)	1(0)	-	0(0)				3ν ₁₀ ℓ = +3	[86007]
	17232.86	(0.10)	1(0)	-	0(0)				3ν ₁₀ ℓ = +1	[86007]
	17233.36	(0.10)	1(0)	-	0(0)				3ν ₁₀ ℓ = +1	[86007]
	17277.010	(0.200)	1(0)	-	0(0)				4ν ₁₀ ℓ = +4	[86020]
	34031.744	(0.010)	2(0)	-	1(0)				1ν ₅	[80038]
	34032.416	(0.010)	2(1)	-	1(1)				1ν ₅	[80038]
	34182.762	(0.005)	2(1)	-	1(1)					[80038]
	34183.413	(0.005)	2(0)	-	1(0)					[80038]
	34187.238	(0.050)	2(+1)	-	1(+1)				1ν ₉ ℓ = +1	[84032]
	34202.900	(0.050)	2(+1)	-	1(+1)				1ν ₉ ℓ = -1	[84032]
	34204.130	(0.050)	2(0)	-	1(0)				1ν ₉ ℓ = +1	[84032]
	34223.401	(0.050)	2(+1)	-	1(+1)				1ν ₉ ℓ = +1	[84032]
	34227.592	(0.200)	2(+1)	-	1(+1)				2ν ₉ ℓ = +2	[86019]
	34246.269	(0.050)	2(+1)	-	1(+1)				1ν ₁₀ ℓ = +1	[84032]
	34277.184	(0.050)	2(+1)	-	1(+1)				1ν ₁₀ ℓ = -1	[84032]
	34279.161	(0.050)	2(0)	-	1(0)				1ν ₁₀ ℓ = +1	[84032]
	34313.523	(0.050)	2(+1)	-	1(+1)				1ν ₁₀ ℓ = +1	[84032]
	34369.481	(0.100)	2(+1)	-	1(+1)				2ν ₁₀ ℓ = -2	[85015]
	34373.015	(0.100)	2(0)	-	1(0)				2ν ₁₀ ℓ = +2	[85015]
	34373.759	(0.100)	2(1)	-	1(1)				2ν ₁₀ ℓ = 0	[85015]
	34374.513	(0.100)	2(0)	-	1(0)				2ν ₁₀ ℓ = 0	[85015]
	34402.40	(0.10)	2(-1)	-	1(-1)				3ν ₁₀ ℓ = -1	[86007]
	34459.79	(0.10)	2(+1)	-	1(+1)				3ν ₁₀ ℓ = -3	[86007]
	34464.81	(0.10)	2(0)	-	1(0)				3ν ₁₀ ℓ = +3	[86007]
	34465.50	(0.10)	2(0)	-	1(0)				3ν ₁₀ ℓ = +1	[86007]
	34467.96	(0.10)	2(+1)	-	1(+1)				3ν ₁₀ ℓ = +3	[86007]
	34536.12	(0.10)	2(1)	-	1(1)				3ν ₁₀ ℓ = 1	[86007]
	34547.348	(0.200)	2(+1)	-	1(+1)				4ν ₁₀ ℓ = +2	[86020]
	34553.348	(0.200)	2(0)	-	1(0)				4ν ₁₀ ℓ = +4	[86020]
	34556.808	(0.200)	2(-1)	-	1(-1)				4ν ₁₀ ℓ = +2	[86020]
	34558.234	(0.200)	2(+1)	-	1(+1)				4ν ₁₀ ℓ = 0	[86020]
	34561.225	(0.200)	2(0)	-	1(0)				4ν ₁₀ ℓ = 0	[86020]
	34561.315	(0.200)	2(+1)	-	1(+1)				4ν ₁₀ ℓ = +4	[86020]
	34561.876	(0.200)	2(0)	-	1(0)				4ν ₁₀ ℓ = +2	[86020]
	51271.000	(0.030)	3(2)	-	2(2)					[84032]
	51273.980	(0.030)	3(1)	-	2(1)					[84032]
	51274.947	(0.030)	3(0)	-	2(0)					[84032]
	51280.668	(0.050)	3(+1)	-	2(+1)				1ν ₉ ℓ = +1	[84032]
	51304.220	(0.050)	3(+1)	-	2(+1)				1ν ₉ ℓ = -1	[84032]
	51306.073	(0.050)	3(0)	-	2(0)				1ν ₉ ℓ = +1	[84032]
	51307.609	(0.050)	3(+2)	-	2(+2)				1ν ₉ ℓ = +1	[84032]
	51322.344	(0.200)	3(-2)	-	2(-2)				2ν ₉ ℓ = +2	[86019]
	51330.025	(0.200)	3(-1)	-	2(-1)				2ν ₉ ℓ = +2	[86019]
	51334.949	(0.050)	3(+1)	-	2(+1)				1ν ₉ ℓ = +1	[84032]
	51340.980	(0.200)	3(+1)	-	2(+1)				2ν ₉ ℓ = +2	[86019]
	51343.854	(0.200)	3(+2)	-	2(+2)				2ν ₉ ℓ = +2	[86019]
	51369.214	(0.050)	3(+1)	-	2(+1)				1ν ₁₀ ℓ = +1	[84032]
	51410.612	(0.050)	3(+2)	-	2(+2)				1ν ₁₀ ℓ = -1	[84032]
	51415.471	(0.050)	3(+1)	-	2(+1)				1ν ₁₀ ℓ = -1	[84032]
	51418.341	(0.050)	3(0)	-	2(0)				1ν ₁₀ ℓ = +1	[84032]
	51418.915	(0.050)	3(+2)	-	2(+2)				1ν ₁₀ ℓ = +1	[84032]
	51469.901	(0.050)	3(+1)	-	2(+1)				1ν ₁₀ ℓ = +1	[84032]
	51547.171	(0.100)	3(-2)	-	2(-1)				2ν ₁₀ ℓ = +2	[85015]
	51553.774	(0.100)	3(+1)	-	2(+1)				2ν ₁₀ ℓ = -2	[85015]
	51560.432	(0.100)	3(1)	-	2(1)				2ν ₁₀ ℓ = 0	[85015]
	51560.785	(0.100)	3(2)	-	2(2)				2ν ₁₀ ℓ = 0	[85015]
	51561.503	(0.100)	3(0)	-	2(0)				2ν ₁₀ ℓ = 0	[85015]
	51563.414	(0.100)	3(+2)	-	2(+2)				2ν ₁₀ ℓ = 0	[85015]
	51602.90	(0.10)	3(-1)	-	2(-1)				3ν ₁₀ ℓ = -1	[86007]
	51680.33	(0.10)	3(+2)	-	2(+2)				3ν ₁₀ ℓ = -3	[86007]
	51689.32	(0.10)	3(+2)	-	2(+2)				3ν ₁₀ ℓ = -1	[86007]

TABLE 12.5. Microwave spectrum of propyne — Continued

C₃H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' K' - J'' K''$	$F' F_1' - F'' F_1''$	Vib. state	Ref.
	51696.73	(0.10)	3(0) - 2(0)		3ν ₁₀ ℓ = +1	[86007]
	51698.18	(0.10)	3(0) - 2(0)		3ν ₁₀ ℓ = +3	[86007]
	51701.34	(0.10)	3(+2) - 2(+2)		3ν ₁₀ ℓ = +1	[86007]
	51701.89	(0.10)	3(+1) - 2(+1)		3ν ₁₀ ℓ = +3	[86007]
	51803.54	(0.10)	3(1) - 2(1)		3ν ₁₀ ℓ = 1	[86007]
	51804.910	(0.200)	3(-2) - 2(-2)		4ν ₁₀ ℓ = +4	[86020]
	51832.710	(0.200)	3(-1) - 2(-1)		4ν ₁₀ ℓ = +2	[86020]
	51836.464	(0.200)	3(+1) - 2(+1)		4ν ₁₀ ℓ = 0	[86020]
	51842.176	(0.200)	3(0) - 2(0)		4ν ₁₀ ℓ = 0	[86020]
	51843.421	(0.200)	3(+1) - 2(+1)		4ν ₁₀ ℓ = +4	[86020]
	51844.724	(0.200)	3(0) - 2(0)		4ν ₁₀ ℓ = +2	[86020]
	51854.655	(0.200)	3(+2) - 2(+2)		4ν ₁₀ ℓ = 0	[86020]
	51870.727	(0.200)	3(+2) - 2(+2)		4ν ₁₀ ℓ = +4	[86020]
	68354.502	(0.005)	4(3) - 3(3)			[78031]
	68361.035	(0.001)	4(2) - 3(2)			[78031]
	68364.956	(0.001)	4(1) - 3(1)			[78031]
	68366.230	(0.030)	4(0) - 3(0)			[69063]
	68373.872	(0.050)	4(+1) - 3(+1)		1ν ₉ ℓ = +1	[84032]
	68384.644	(0.050)	4(+3) - 3(+3)		1ν ₉ ℓ = -1	[84032]
	68394.941	(0.050)	4(+2) - 3(+2)		1ν ₉ ℓ = -1	[84032]
	68405.342	(0.050)	4(+1) - 3(+1)		1ν ₉ ℓ = -1	[84032]
	68406.824	(0.050)	4(+3) - 3(+3)		1ν ₉ ℓ = +1	[84032]
	68407.856	(0.050)	4(0) - 3(0)		1ν ₉ ℓ = +1	[84032]
	68409.668	(0.050)	4(+2) - 3(+2)		1ν ₉ ℓ = +1	[84032]
	68446.336	(0.050)	4(+1) - 3(+1)		1ν ₉ ℓ = +1	[84032]
	68447.100	(0.050)	4(+1) - 3(+1)		2ν ₉ ℓ = 0	[86019]
	68448.633	(0.200)	4(0) - 3(0)		2ν ₉ ℓ = +2	[86019]
	68448.875	(0.050)	4(0) - 3(0)		2ν ₉ ℓ = 0	[86019]
	68491.993	(0.030)	4(+1) - 3(+1)		1ν ₁₀ ℓ = +1	[69063]
	68454.518	(0.200)	4(+1) - 3(+1)		2ν ₉ ℓ = +2	[86019]
	68457.956	(0.200)	4(+2) - 3(+2)		2ν ₉ ℓ = +2	[86019]
	68538.052	(0.030)	4(+3) - 3(+3)		1ν ₁₀ ℓ = -1	[69063]
	68547.148	(0.030)	4(+2) - 3(+2)		1ν ₁₀ ℓ = -1	[69063]
	68553.602	(0.030)	4(+1) - 3(+1)		1ν ₁₀ ℓ = -1	[69063]
	68554.251	(0.030)	4(+3) - 3(+3)		1ν ₁₀ ℓ = +1	[69063]
	68557.333	(0.030)	4(0) - 3(0)		1ν ₁₀ ℓ = +1	[69063]
	68558.447	(0.030)	4(+2) - 3(+2)		1ν ₁₀ ℓ = +1	[69063]
	68626.217	(0.030)	4(+1) - 3(+1)		1ν ₁₀ ℓ = +1	[69063]
	68737.665	(0.100)	4(+1) - 3(+1)		2ν ₁₀ ℓ = -2	[85015]
	68738.533	(0.100)	4(3) - 3(3)		2ν ₁₀ ℓ = 0	[85015]
	68740.904	(0.100)	4(2) - 3(2)		2ν ₁₀ ℓ = 0	[85015]
	68746.134	(0.100)	4(1) - 3(1)		2ν ₁₀ ℓ = 0	[85015]
	68747.724	(0.100)	4(0) - 3(0)		2ν ₁₀ ℓ = 0	[85015]
	68749.992	(0.100)	4(+2) - 3(+2)		2ν ₁₀ ℓ = +2	[85015]
	85431.224	(0.060)	5(4) - 4(4)			[69063]
	85442.528	(0.060)	5(3) - 4(3)			[69063]
	85450.730	(0.060)	5(2) - 4(2)			[69063]
	85455.622	(0.060)	5(1) - 4(1)			[69063]
	85457.272	(0.060)	5(0) - 4(0)			[69063]
	85614.570	(0.060)	5(+1) - 4(+1)		1ν ₁₀ ℓ = +1	[69063]
	85683.174	(0.060)	5(+2) - 4(+2)		1ν ₁₀ ℓ = -1	[69063]
	85684.002	(0.060)	5(+4) - 4(+4)		1ν ₁₀ ℓ = +1	[69063]
	85691.206	(0.060)	5(+1) - 4(+1)		1ν ₁₀ ℓ = -1	[69063]
	85692.374	(0.060)	5(+3) - 4(+3)		1ν ₁₀ ℓ = +1	[69063]
	85695.638	(0.060)	5(0) - 4(0)		1ν ₁₀ ℓ = +1	[69063]
	85697.750	(0.060)	5(+2) - 4(+2)		1ν ₁₀ ℓ = +1	[69063]
	85782.322	(0.060)	5(+1) - 4(+1)		1ν ₁₀ ℓ = +1	[69063]
	102499.110	(0.090)	6(5) - 5(5)			[69063]
	102516.573	(0.090)	6(4) - 5(4)			[69063]
	102530.348	(0.003)	6(3) - 5(3)			[78031]
	102540.145	(0.002)	6(2) - 5(2)			[78031]
	102546.024	(0.001)	6(1) - 5(1)			[78031]
	102547.984	(0.001)	6(0) - 5(0)			[78031]
	102736.158	(0.090)	6(+1) - 5(+1)		1ν ₁₀ ℓ = +1	[69063]
	102766.158	(0.090)	6(+5) - 5(+5)		1ν ₁₀ ℓ = -1	[69063]
	102787.743	(0.090)	6(+4) - 5(+4)		1ν ₁₀ ℓ = -1	[69063]
	102805.311	(0.090)	6(+3) - 5(+3)		1ν ₁₀ ℓ = -1	[69063]

TABLE 12.5. Microwave spectrum of propyne — Continued

C₃H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' K' - J'' K''$	$F' F_1' - F'' F_1''$	Vib. state	Ref.
	102818.949	(0.090)	6(+2) - 5(+2)		1ν ₁₀ ℓ = -1	[69063]
	102820.305	(0.090)	6(+4) - 5(+4)		1ν ₁₀ ℓ = +1	[69063]
	102828.543	(0.090)	6(+1) - 5(+1)		1ν ₁₀ ℓ = -1	[69063]
	102830.418	(0.090)	6(+3) - 5(+3)		1ν ₁₀ ℓ = +1	[69063]
	102833.604	(0.090)	6(0) - 5(0)		1ν ₁₀ ℓ = +1	[69063]
	102837.186	(0.090)	6(+2) - 5(+2)		1ν ₁₀ ℓ = +1	[69063]
	102938.040	(0.090)	6(+1) - 5(+1)		1ν ₁₀ ℓ = +1	[69063]
	119556.066	(0.060)	7(6) - 6(6)			[69063]
	119581.168	(0.060)	7(5) - 6(5)			[69063]
	119601.726	(0.060)	7(4) - 6(4)			[69063]
	119617.671	(0.005)	7(3) - 6(3)			[78031]
	119629.101	(0.002)	7(2) - 6(2)			[78031]
	119635.958	(0.002)	7(1) - 6(1)			[78031]
	119638.244	(0.001)	7(0) - 6(0)			[78031]
	119858.368	(0.060)	7(+1) - 6(+1)		1ν ₁₀ ℓ = +1	[69063]
	119892.576	(0.060)	7(+5) - 6(+5)		1ν ₁₀ ℓ = -1	[69063]
	119917.696	(0.060)	7(+4) - 6(+4)		1ν ₁₀ ℓ = -1	[69063]
	119919.060	(0.060)	7(+6) - 6(+6)		1ν ₁₀ ℓ = +1	[69063]
	119938.214	(0.060)	7(+3) - 6(+3)		1ν ₁₀ ℓ = -1	[69063]
	119939.884	(0.060)	7(+5) - 6(+5)		1ν ₁₀ ℓ = +1	[69063]
	119954.032	(0.060)	7(+2) - 6(+2)		1ν ₁₀ ℓ = -1	[69063]
	119956.112	(0.060)	7(+4) - 6(+4)		1ν ₁₀ ℓ = +1	[69063]
	119965.098	(0.060)	7(+1) - 6(+1)		1ν ₁₀ ℓ = -1	[69063]
	119968.032	(0.060)	7(+3) - 6(+3)		1ν ₁₀ ℓ = +1	[69063]
	119970.604	(0.060)	7(0) - 6(0)		1ν ₁₀ ℓ = +1	[69063]
	119976.230	(0.060)	7(+2) - 6(+2)		1ν ₁₀ ℓ = +1	[69063]
	120093.174	(0.060)	7(+1) - 6(+1)		1ν ₁₀ ℓ = +1	[69063]
	136600.15	(0.30)	8(7) - 7(7)			[57014]
	136634.03	(0.30)	8(6) - 7(6)			[57014]
	136662.74	(0.30)	8(5) - 7(5)			[57014]
	136686.19	(0.30)	8(4) - 7(4)			[57014]
	136704.502	(0.002)	8(3) - 7(3)			[78031]
	136717.560	(0.002)	8(2) - 7(2)			[78031]
	136725.397	(0.001)	8(1) - 7(1)			[78031]
	136728.010	(0.001)	8(0) - 7(0)			[78031]
	153629.472	(0.050)	9(8) - 8(8)			[78031]
	153673.424	(0.030)	9(7) - 8(7)			[78031]
	153711.520	(0.030)	9(6) - 8(6)			[78031]
	153743.800	(0.030)	9(5) - 8(5)			[78031]
	153770.224	(0.030)	9(4) - 8(4)			[78031]
	153790.769	(0.002)	9(3) - 8(3)			[78031]
	153805.458	(0.002)	9(2) - 8(2)			[78031]
	153814.273	(0.001)	9(1) - 8(1)			[78031]
	153817.212	(0.001)	9(0) - 8(0)			[78031]
	170746.05	(0.35)	10(7) - 9(7)			[57014]
	170788.29	(0.35)	10(6) - 9(6)			[57014]
	170824.13	(0.35)	10(5) - 9(5)			[57014]
	170853.50	(0.35)	10(4) - 9(4)			[57014]
	170876.27	(0.35)	10(3) - 9(3)			[57014]
	170892.59	(0.35)	10(2) - 9(2)			[57014]
	170902.37	(0.35)	10(1) - 9(1)			[57014]
	170905.66	(0.35)	10(0) - 9(0)			[57014]
	187763.96	(0.40)	11(8) - 10(8)			[57014]
	187817.95	(0.40)	11(7) - 10(7)			[57014]
	187864.42	(0.40)	11(6) - 10(6)			[57014]
	187903.96	(0.40)	11(5) - 10(5)			[57014]
	187936.34	(0.40)	11(4) - 10(4)			[57014]
	187961.41	(0.40)	11(3) - 10(3)			[57014]
	187979.34	(0.40)	11(2) - 10(2)			[57014]
	187990.02	(0.40)	11(1) - 10(1)			[57014]
	187993.69	(0.40)	11(0) - 10(0)			[57014]
	204690.354	(0.050)	12(10) - 11(10)			[78031]
	204764.348	(0.050)	12(9) - 11(9)			[78031]
	204889.088	(0.040)	12(7) - 11(7)			[78031]
	204939.908	(0.050)	12(6) - 11(6)			[78031]
	204982.869	(0.050)	12(5) - 11(5)			[78031]
	205018.080	(0.050)	12(4) - 11(4)			[78031]

TABLE 12.5. Microwave spectrum of propyne — Continued

C₃H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' K' - J'' K''$	$F' F_1' - F'' F_1''$	Vib. state	Ref.
	205065.015	(0.050)	12(2) - 11(2)			[78031]
	205076.775	(0.050)	12(1) - 11(1)			[78031]
	205080.660	(0.050)	12(0) - 11(0)			[78031]
	221824.368	(0.050)	13(9) - 12(9)			[78031]
	221959.38	(0.45)	13(7) - 12(7)			[57014]
	222014.448	(0.050)	13(6) - 12(6)			[78031]
	222060.95	(0.45)	13(5) - 12(5)			[57014]
	222099.05	(0.45)	13(4) - 12(4)			[57014]
	222128.808	(0.050)	13(3) - 12(3)			[78031]
	222149.80	(0.45)	13(2) - 12(2)			[57014]
	222162.46	(0.45)	13(1) - 12(1)			[57014]
	222166.790	(0.005)	13(0) - 12(0)			[78031]
	238484.892	(0.090)	14(13) - 13(13)			[78031]
	238597.896	(0.060)	14(12) - 13(12)			[78031]
	238883.496	(0.060)	14(9) - 13(9)			[78031]
	238960.752	(0.060)	14(8) - 13(8)			[78031]
	239088.144	(0.030)	14(6) - 13(6)			[78031]
	239138.04	(0.50)	14(5) - 13(5)			[78031]
	239179.248	(0.030)	14(4) - 13(4)			[78031]
	239211.216	(0.020)	14(3) - 14(3)			[78031]
	239234.011	(0.020)	14(2) - 13(2)			[78031]
	239247.727	(0.007)	14(1) - 13(1)			[78031]
	239252.296	(0.003)	14(0) - 13(0)			[78031]
¹³ CH ₃ CCH	33252.22	(0.03)	2(1) - 1(1)			[50022]
	33252.88	(0.03)	2(0) - 1(0)			[50022]
	66503.98	(0.03)	4(1) - 3(1)			[78031]
	99710.02	(0.03)	6(5) - 5(5)			[78031]
	99726.79	(0.03)	6(4) - 5(4)			[78031]
	99739.77	(0.03)	6(3) - 5(3)			[78031]
	99749.10	(0.03)	6(2) - 5(2)			[78031]
	99754.70	(0.03)	6(1) - 5(1)			[78031]
	99756.55	(0.03)	6(0) - 5(0)			[78031]
	116362.10	(0.03)	7(3) - 6(3)			[78031]
	116372.96	(0.03)	7(2) - 6(2)			[78031]
	116379.48	(0.03)	7(1) - 6(1)			[78031]
	116381.65	(0.03)	7(0) - 6(0)			[78031]
	132916.94	(0.03)	8(6) - 7(6)			[78031]
	132944.31	(0.03)	8(5) - 7(5)			[78031]
	132966.54	(0.03)	8(4) - 7(4)			[78031]
	132983.87	(0.03)	8(3) - 7(3)			[78031]
	132996.26	(0.03)	8(2) - 7(2)			[78031]
	133003.74	(0.03)	8(1) - 7(1)			[78031]
	133006.22	(0.03)	8(0) - 7(0)			[78031]
	149529.91	(0.03)	9(6) - 8(6)			[78031]
	149585.65	(0.03)	9(4) - 8(4)			[78031]
	149605.14	(0.03)	9(3) - 8(3)			[78031]
	149619.10	(0.03)	9(2) - 8(2)			[78031]
	149627.46	(0.03)	9(1) - 8(1)			[78031]
	149630.26	(0.03)	9(0) - 8(0)			[78031]
	232389.79	(0.03)	14(9) - 13(9)			[78031]
	232463.11	(0.03)	14(8) - 13(8)			[78031]
	232584.12	(0.03)	14(6) - 13(6)			[78031]
	232631.81	(0.03)	14(5) - 13(5)			[78031]
	232670.76	(0.03)	14(4) - 13(4)			[78031]
	232701.07	(0.03)	14(3) - 13(3)			[78031]
	232722.70	(0.03)	14(2) - 13(2)			[78031]
	232735.78	(0.03)	14(1) - 13(1)			[78031]
	232740.07	(0.03)	14(0) - 13(0)			[78031]
CH ₃ ¹³ CCH	34168.47	(0.10)	2(1) - 1(1)			[50022]
	34169.13	(0.10)	2(0) - 1(0)			[50022]
	68326.19	(0.03)	4(3) - 3(3)			[78031]
	68332.72	(0.03)	4(2) - 3(2)			[78031]
	68336.61	(0.03)	4(1) - 3(1)			[78031]
	102456.65	(0.03)	6(5) - 5(5)			[78031]
	102474.22	(0.03)	6(4) - 5(4)			[78031]
	102487.86	(0.03)	6(3) - 5(3)			[78031]
	102497.64	(0.03)	6(2) - 5(2)			[78031]

TABLE 12.5. Microwave spectrum of propyne — Continued

C₃H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' K' - J'' K''$	$F' F'_1 - F'' F''_1$	Vib. state	Ref.
	102503.46	(0.03)	6(1) - 5(1)			[78031]
	102505.41	(0.03)	6(1) - 5(1)			[78031]
	119568.11	(0.03)	7(3) - 6(3)			[78031]
	119586.37	(0.03)	8(1) - 6(1)			[78031]
	119588.64	(0.03)	8(0) - 6(0)			[78031]
	136577.67	(0.03)	8(6) - 7(6)			[78031]
	136606.29	(0.03)	8(5) - 7(5)			[78031]
	136629.64	(0.03)	8(4) - 7(4)			[78031]
	136647.86	(0.03)	8(3) - 7(3)			[78031]
	136660.87	(0.03)	8(2) - 7(2)			[78031]
	136668.71	(0.03)	8(1) - 7(1)			[78031]
	136671.34	(0.03)	8(0) - 7(0)			[78031]
	153648.06	(0.03)	9(6) - 8(6)			[78031]
	153680.22	(0.03)	9(5) - 8(5)			[78031]
	153706.59	(0.03)	9(4) - 8(4)			[78031]
	153727.01	(0.03)	9(3) - 8(3)			[78031]
	153741.68	(0.03)	9(2) - 8(2)			[78031]
	153750.47	(0.03)	9(1) - 8(1)			[78031]
	153753.37	(0.03)	9(0) - 8(0)			[78031]
	204680.53	(0.03)	12(9) - 11(9)			[78031]
	204746.49	(0.03)	12(8) - 11(8)			[78031]
	204855.33	(0.03)	12(6) - 11(6)			[78031]
	204898.17	(0.03)	12(5) - 11(5)			[78031]
	204933.24	(0.03)	12(4) - 11(4)			[78031]
	204960.52	(0.03)	12(3) - 11(3)			[78031]
	204980.07	(0.03)	12(2) - 11(2)			[78031]
	204991.68	(0.03)	12(1) - 11(1)			[78031]
	204995.65	(0.03)	12(0) - 11(0)			[78031]
	221653.61	(0.03)	13(10) - 12(10)			[78031]
	221733.38	(0.03)	13(9) - 12(9)			[78031]
	221804.98	(0.03)	13(8) - 12(8)			[78031]
	221868.10	(0.03)	13(7) - 12(7)			[78031]
	221922.88	(0.03)	13(6) - 12(6)			[78031]
	221969.18	(0.03)	13(5) - 12(5)			[78031]
	222036.66	(0.03)	13(3) - 12(3)			[78031]
	222057.79	(0.03)	13(2) - 12(2)			[78031]
	222070.52	(0.03)	13(1) - 12(1)			[78031]
	222074.70	(0.03)	13(0) - 12(0)			[78031]
	239152.94	(0.03)	14(0) - 13(0)			[78031]
CH ₃ C ¹³ CH	33160.35	(0.03)	2(1) - 1(1)			[50022]
	33160.94	(0.03)	2(0) - 1(0)			[50022]
	66310.05	(0.03)	4(3) - 3(3)			[78031]
	66320.01	(0.03)	4(1) - 3(1)			[78031]
	99433.95	(0.03)	6(5) - 5(5)			[78031]
	99450.75	(0.03)	6(4) - 5(4)			[78031]
	99463.77	(0.03)	6(3) - 5(3)			[78031]
	99473.07	(0.03)	6(2) - 5(2)			[78031]
	99478.69	(0.03)	6(1) - 5(1)			[78031]
	99480.52	(0.03)	6(0) - 5(0)			[78031]
	116040.13	(0.03)	7(3) - 6(3)			[78031]
	116051.01	(0.03)	7(2) - 6(2)			[78031]
	116057.53	(0.03)	7(1) - 6(1)			[78031]
	116059.70	(0.03)	7(0) - 6(0)			[78031]
	132548.86	(0.03)	8(6) - 7(6)			[78031]
	132576.16	(0.03)	8(5) - 7(5)			[78031]
	132598.52	(0.03)	8(4) - 7(4)			[78031]
	132615.92	(0.03)	8(3) - 7(3)			[78031]
	132628.35	(0.03)	8(2) - 7(2)			[78031]
	132635.81	(0.03)	8(1) - 7(1)			[78031]
	132638.26	(0.03)	8(0) - 7(0)			[78031]
	149115.84	(0.03)	9(6) - 8(6)			[78031]
	149146.51	(0.03)	9(5) - 8(5)			[78031]
	149171.62	(0.03)	9(4) - 8(4)			[78031]
	149191.26	(0.03)	9(3) - 8(3)			[78031]
	149205.18	(0.03)	9(2) - 8(2)			[78031]
	149213.55	(0.03)	9(1) - 8(1)			[78031]
	149216.35	(0.03)	9(0) - 8(0)			[78031]

TABLE 12.5. Microwave spectrum of propyne — Continued

C₃H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' K' - J'' K''$	$F' F'_i - F'' F''_i$	Vib. state	Ref.
	215324.65	(0.03)	13(7) - 12(7)			[78031]
	215376.95	(0.03)	13(6) - 12(6)			[78031]
	215421.31	(0.03)	13(5) - 12(5)			[78031]
	215457.58	(0.03)	13(4) - 12(4)			[78031]
	215485.82	(0.03)	13(3) - 12(3)			[78031]
	215505.96	(0.03)	13(2) - 12(2)			[78031]
	215518.12	(0.03)	13(1) - 12(1)			[78031]
	215522.17	(0.03)	13(0) - 12(0)			[78031]
	231745.61	(0.03)	14(9) - 13(9)			[78031]
	231819.11	(0.03)	14(8) - 13(8)			[78031]
	231884.04	(0.03)	14(7) - 13(7)			[78031]
	231940.37	(0.03)	14(6) - 13(6)			[78031]
	232027.20	(0.03)	14(4) - 13(4)			[78031]
	232057.54	(0.03)	14(3) - 13(3)			[78031]
	232079.26	(0.03)	14(2) - 13(2)			[78031]
	232092.26	(0.03)	14(1) - 13(1)			[78031]
	232096.61	(0.03)	14(0) - 13(0)			[78031]
CH ₃ CCD	15576.309	(0.001)	1(0) - 0(0)	2 5/2 - 1 5/2		[82035]
	15576.317	(0.001)	1(0) - 0(0)	2 3/2 - 1 3/2		[82035]
	15576.321	(0.001)	1(0) - 0(0)	2 7/2 - 1 5/2		[82035]
	15576.328	(0.001)	1(0) - 0(0)	2 1/2 - 1 1/2		[82035]
	15576.379	(0.001)	1(0) - 0(0)	1 1/2 - 1 1/2		[82035]
	15576.385	(0.001)	1(0) - 0(0)	1 5/2 - 1 5/2		[82035]
	15576.393	(0.001)	1(0) - 0(0)	1 3/2 - 1 3/2		[82035]
	31152.00	(0.10)	2(1) - 1(1)			[50022]
	31152.56	(0.10)	2(0) - 1(0)			[50022]
	46725.32	(0.10)	3(2) - 2(2)			[55018]
	46727.86	(0.10)	3(1) - 2(1)			[55018]
	46728.72	(0.10)	3(0) - 2(0)			[55018]
CD ₃ CCH	14711.523	(0.001)	1(0) - 0(0)	1 - 3		[82035]
	14711.531	(0.001)	1(0) - 0(0)	2 - 3		[82035]
	14711.566	(0.001)	1(0) - 0(0)	4 - 3		[82035]
	29422.50	(0.10)	2(1) - 1(1)			[55018]
	29422.89	(0.10)	2(0) - 1(0)			[55018]
	44131.76	(0.10)	3(2) - 2(2)			[55018]
	44133.62	(0.10)	3(1) - 2(1)			[55018]
	44134.19	(0.10)	3(0) - 2(0)			[55018]
CD ₂ CCD	58845.565	(0.015)	4(0) - 3(0)			[70029]
	26936.87	(0.10)	2(1) - 1(1)			[50022]
	26937.24	(0.10)	2(0) - 1(0)			[50022]
	40403.60	(0.10)	3(2) - 2(2)			[55018]
	40405.21	(0.10)	3(1) - 2(1)			[55018]
	40405.75	(0.10)	3(0) - 2(0)			[55018]
CH ₂ DCCH	16181.12	(0.10)	1(0, 1) - 0(0, 0)			[55018]
	32231.44	(0.10)	2(1, 2) - 1(1, 1)			[55018]
	32362.08	(0.10)	2(0, 2) - 1(0, 1)			[55018]
	32491.86	(0.10)	2(1, 1) - 1(1, 0)			[55018]
	48346.90	(0.10)	3(1, 3) - 2(1, 2)			[55018]
	48539.96	(0.10)	3(2, 2) - 2(2, 1)			[55018]
	48540.33	(0.10)	3(2, 1) - 2(2, 0)			[55018]
	48542.62	(0.10)	3(0, 3) - 2(0, 2)			[55018]
	48737.52	(0.10)	3(1, 2) - 2(1, 1)			[55018]
CHD ₂ CCH	30658.07	(0.10)	2(1, 2) - 1(1, 1)			[55018]
	30793.13	(0.10)	2(0, 2) - 1(0, 1)			[55018]
	30927.55	(0.10)	2(1, 1) - 1(1, 0)			[55018]
	45986.74	(0.10)	3(1, 3) - 2(1, 2)			[55018]
	46186.84	(0.10)	3(2, 2) - 2(2, 1)			[55018]
	46187.46	(0.10)	3(2, 1) - 2(2, 0)			[55018]
	46189.01	(0.10)	3(0, 3) - 2(0, 2)			[55018]
	46391.00	(0.10)	3(1, 2) - 2(1, 1)			[55018]
CH ₂ DCCD	29436.09	(0.10)	2(1, 2) - 1(1, 1)			[55018]
	29545.33	(0.10)	2(0, 2) - 1(0, 1)			[55018]
	29653.70	(0.10)	2(1, 1) - 1(1, 0)			[55018]
	44154.10	(0.10)	3(1, 3) - 2(1, 2)			[55018]
	44315.24	(0.10)	3(2, 2) - 2(2, 1)			[55018]
	44315.50	(0.10)	3(2, 1) - 2(2, 0)			[55018]
	44317.72	(0.10)	3(0, 3) - 2(0, 2)			[55018]

TABLE 12.5. Microwave spectrum of propyne — Continued

C₃H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' K' - J'' K''$	$F' F_1' - F'' F_1''$	Vib. state	Ref.
CHD ₂ CCD	44480.44	(0.10)	3(1, 2) - 2(1, 1)			[55018]
	28042.28	(0.10)	2(1, 2) - 1(1, 1)			[55018]
	28155.14	(0.10)	2(0, 2) - 1(0, 1)			[55018]
	28267.33	(0.10)	2(1, 1) - 1(1, 0)			[55018]
	42063.15	(0.10)	3(1, 3) - 2(1, 2)			[55018]
	42230.22	(0.10)	3(2, 2) - 2(2, 1)			[55018]
	42230.61	(0.10)	3(2, 1) - 2(2, 0)			[55018]
	42232.30	(0.10)	3(0, 3) - 2(0, 2)			[55018]
	42400.70	(0.10)	3(1, 2) - 2(1, 1)			[55018]

Table 13.1. Molecular constants for the ground state of propylene from fitting internal rotation and the A state alone.

Parameter	Fit to A and E States Value ^a	Parameter	Fit to A State Value ^b
A (MHz)	46280.33(23)	A'' (MHz)	46290.523(204)
B (MHz)	9305.238(25)	B'' (MHz)	9305.354(25)
C (MHz)	8134.214(23)	C'' (MHz)	8134.314(21)
Δ_J (MHz)	0.00655(83)	τ_1 (MHz)	0.0174(352)
Δ_{JK} (MHz)	-0.0264(84)	τ_2 (MHz)	-0.0141(60)
Δ_K (MHz)	0.479(49)	τ_3 (MHz)	1.037(130)
δ_J (MHz)	0.001238(312)	τ_{aaaa} (MHz)	-2.794(154)
δ_K (MHz)	-0.0291(22)	τ_{bbbb} (MHz)	-0.0348(23)
I_α (u Å ²)	3.16	τ_{cccc} (MHz)	-0.0151(20)
θ	24.84°		
V_3 (cm ⁻¹)	687.87(7)		

^aUncertainties 1 σ .^bUncertainties 2 σ .

Table 13.2. Dipole moment and Zeeman constants for propylene.

Parameter	Value
<u>Electric Dipole Moment</u> [57015]	
μ_a	0.360(1) D
μ_b	0.05(2) D
<u>Zeeman Parameters</u> [69065]	
g_{aa}	-0.0789(6) μ_N
g_{bb}	-0.0424(4) μ_N
g_{cc}	+0.0107(5) μ_N
$2\chi_{aa}-\chi_{bb}-\chi_{cc}$	-0.74(3) $\times 10^{-6}$ erg/G ² ·mol
$-\chi_{aa}+2\chi_{bb}-\chi_{cc}$	+13.4(5) $\times 10^{-6}$ erg/G ² ·mol
Q_{aa}	0.6(3) $\times 10^{-26}$ esu·cm ²
Q_{bb}	2.9(5) $\times 10^{-26}$ esu·cm ²
Q_{cc}	-3.5(7) $\times 10^{-26}$ esu·cm ²

Table 13.3. Molecular constants for propylene (CH₃CH=CH₂) in excited torsional states.

Parameter	v=1 State	v=2 State
A (MHz)	46280. ^a	46280. ^a
B (MHz)	9293.902	9282.001
C (MHz)	8138.561	8142.708
I_α (u Å ²)	3.160 ^a	3.160 ^a
θ	(24.8°)	(24.6°)
λ_a	0.90762	0.90898
λ_b	0.41980	0.41684
V_3 (cm ⁻¹)	697.48	703.65
s	43.652	44.005
F (cm ⁻¹)	7.1010	7.1063
Reference	[66045]	[66045]

^aValues fixed in the analysis.

Table 13.4. Molecular constants for the deuterated propylene species t-CHDCHCH₃ and CH₂CDCH₃ in the ground and excited torsional states. [66045]

Parameter	t-CHDCHCH ₃		CH ₂ CDCH ₃	
	v=0	v=1	v=0	v=1
A (MHz)	45912.6 ^a	45912.6 ^a	38154.2 ^a	38154.2 ^a
B (MHz)	8548.01	8538.45	9301.81	9290.65
C (MHz)	7542.20	7546.21	7837.18	7839.64
I _α (uÅ ²)	3.16 ^a	3.16 ^a	3.16 ^a	3.16 ^a
λ _a	0.924	0.913	0.897	0.909
λ _b	0.381	0.408	0.442	0.415
V ₃ (cm ⁻¹)	691.	699.1	688.	698.9
s	43.0	43.78	45.6	46.19
F (cm ⁻¹)	7.144	7.096	6.697	6.731

^aFixed value.

Table 13.5. Rotational constants for substituted isotopic forms of propylene.

Species	A (GHz)	B (MHz)	C (MHz)	Reference
¹³ CH ₂ CHCH ₃	46.00(20)	9048.33(5)	8430.84(5)	[61013]
CH ₂ ¹³ CHCH ₃	45.30(20)	9304.15(5)	8107.14(5)	[61013]
CH ₂ CH ¹³ CH ₃	46.17(20)	9047.94(5)	7932.98(5)	[61013]
c-CHDCHCH ₃	40.22(20)	9040.09(5)	7729.65(5)	[61013]
s-CH ₂ CHCH ₂ D	40.59(20)	9066.99(5)	7765.98(5)	[61013]
a-CH ₂ CHCH ₂ D	43.26(20)	8659.02(5)	7718.11(5)	[61013]
s-CH ₂ CDCH ₂ D	34.06	9058.28	7483.72	[66044]
t-CDHCDCH ₃	33.71	9038.74	7451.01	[66044]
c-CDHCHCH ₂ D	35.71	8821.61	7397.33	[66044]
a-CH ₂ CDCH ₂ D	36.18	8654.53	7449.49	[66044]
c-CHDCDCH ₃	37.96	8546.43	7289.36	[66044]
a-CH ₂ CHCD ₂ H	38.22	8469.44	7395.45	[66044]
ca-CDHCHCH ₂ D	38.20	8411.37	7340.45	[66044]
CD ₂ CHCH ₃	39.82	8347.03	7203.75	[66044]
ts-CHDCHCH ₂ D	40.36	8324.23	7210.10	[66044]
s-CH ₂ CHCHD ₂	39.73	8111.44	7370.87	[66044]
ta-CHDCHCH ₂ D	43.04	7976.26	7164.02	[66044]

TABLE 13.6. Microwave spectrum of propylene

C₃H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$	-	$J''(K_{-1}, K_{+1})$	v_1	Sym.	Ref.
CH ₂ CHCH ₃	8586.71	(0.20)	9(2, 7)	-	9(2, 8)	0	A	[66045]
	8588.64	(0.20)	9(2, 7)	-	9(2, 8)	0	E	[66045]
	9409.09	(0.20)	6(2, 4)	-	7(1, 7)	0	E	[66045]
	9447.61	(0.20)	6(2, 4)	-	7(1, 7)	0	A	[66045]
	9845.22	(0.20)	16(3, 13)	-	16(3, 14)	0	A	[66045]
	9848.63	(0.20)	16(3, 13)	-	16(3, 14)	0	E	[66045]
	11707.32	(0.20)	4(1, 3)	-	4(1, 4)	0	E	[66045]
	11708.48	(0.20)	4(1, 3)	-	4(1, 4)	0	A	[66045]
	12592.45	(0.20)	10(2, 8)	-	10(2, 9)	0	A	[66045]
	12594.41	(0.20)	10(2, 8)	-	10(2, 9)	0	E	[66045]
	13687.19	(0.20)	17(3, 14)	-	17(3, 15)	0	A	[66045]
	13691.20	(0.20)	17(3, 14)	-	17(3, 15)	0	E	[66045]
	16367.68	(0.20)	3(0, 3)	-	2(1, 2)	0	A	[66045]
	16382.24	(0.20)	3(0, 3)	-	2(1, 2)	0	E	[66045]
	16901.20	(0.20)	4(2, 3)	-	5(1, 4)	0	A	[66045]
	16856.49	(0.20)	4(2, 3)	-	5(1, 4)	0	E	[66045]
	17228.89	(0.20)	1(0, 1)	-	0(0, 0)	2	E	[66045]
	17429.51	(0.20)	1(0, 1)	-	0(0, 0)	1	A	[66045]
	17434.19	(0.20)	1(0, 1)	-	0(0, 0)	1	E	[66045]
	17439.439	(0.200)	1(0, 1)	-	0(0, 0)	0	A	[66045]
	17439.439	(0.200)	1(0, 1)	-	0(0, 0)	0	E	[66045]
	17468.52	(0.20)	1(0, 1)	-	0(0, 0)	2	A	[66045]
	17553.02	(0.20)	5(1, 4)	-	5(1, 5)	0	E	[66045]
	17554.97	(0.20)	5(1, 4)	-	5(1, 5)	0	A	[66045]
	17688.22	(0.20)	11(2, 9)	-	11(2, 10)	0	A	[66045]
	17690.37	(0.20)	11(2, 9)	-	11(2, 10)	0	E	[66045]
	18550.81	(0.20)	18(3, 15)	-	18(3, 16)	0	A	[66045]
	18555.61	(0.20)	18(3, 15)	-	18(3, 16)	0	E	[66045]
	21594.51	(0.20)	5(2, 3)	-	6(1, 6)	0	E	[66045]
	21632.43	(0.20)	5(2, 3)	-	6(1, 6)	0	A	[66045]
	23954.23	(0.20)	12(2, 10)	-	12(2, 11)	0	A	[66045]
	23956.64	(0.20)	12(2, 10)	-	12(2, 11)	0	E	[66045]
	24555.02	(0.20)	6(1, 5)	-	6(1, 6)	0	E	[66045]
	24556.41	(0.20)	19(3, 16)	-	19(3, 17)	0	A	[66045]
	24557.85	(0.20)	6(1, 5)	-	6(1, 6)	0	A	[66045]
	24562.05	(0.20)	19(3, 16)	-	19(3, 17)	0	E	[66045]
	25149.89	(0.20)	7(1, 6)	-	6(2, 5)	0	A	[66045]
	25187.87	(0.20)	7(1, 6)	-	6(2, 5)	0	E	[66045]
	31438.71	(0.20)	13(2, 11)	-	13(2, 12)	0	A	[66045]
	31441.25	(0.20)	13(2, 11)	-	13(2, 12)	0	E	[66045]
	32698.96	(0.20)	7(1, 6)	-	7(1, 7)	0	E	[66045]
	32702.89	(0.20)	7(1, 6)	-	7(1, 7)	0	A	[66045]
	33707.783	(0.200)	2(1, 2)	-	1(1, 1)	0	A	[66045]
	33708.23	(0.20)	2(1, 2)	-	1(1, 1)	0	E	[66045]
	33708.48	(0.20)	2(1, 2)	-	1(1, 1)	1	A	[66045]
	33742.16	(0.20)	2(1, 2)	-	1(1, 1)	2	A	[66045]
	34087.90	(0.20)	2(1, 2)	-	1(1, 1)	1	E	[66045]
	34462.18	(0.20)	2(0, 2)	-	1(0, 1)	2	E	[66045]
	34832.16	(0.20)	2(0, 2)	-	1(0, 1)	1	A	[66045]
	34841.70	(0.20)	2(0, 2)	-	1(0, 1)	1	E	[66045]
	34851.335	(0.200)	2(0, 2)	-	1(0, 1)	0	A	[66045]
	34851.335	(0.200)	2(0, 2)	-	1(0, 1)	0	E	[66045]
	34865.35	(0.20)	2(1, 1)	-	1(1, 0)	2	E	[66045]
	34912.42	(0.20)	2(0, 2)	-	1(0, 1)	2	A	[66045]
	35003.09	(0.20)	2(1, 1)	-	1(1, 0)	2	E	[66045]
	35649.85	(0.20)	2(1, 1)	-	1(1, 0)	1	E	[66045]
	36011.62	(0.20)	2(1, 1)	-	1(1, 0)	1	A	[66045]
36049.233	(0.200)	2(1, 1)	-	1(1, 0)	0	E	[66045]	
36050.132	(0.200)	2(1, 1)	-	1(1, 0)	0	A	[66045]	
36112.68	(0.20)	2(1, 1)	-	1(1, 0)	2	A	[66045]	
¹³ CH ₂ CHCH ₃	32841.16	(0.10)	2(1, 2)	-	1(1, 1)	0	A	[61031]
	33933.42	(0.10)	2(0, 2)	-	1(0, 1)	0	A	[61031]
	35075.17	(0.10)	2(1, 1)	-	1(1, 0)	0	E	[61031]
CH ₂ ¹³ CHCH ₃	35076.09	(0.10)	2(1, 1)	-	1(1, 0)	0	A	[61031]
	17411.29	(0.03)	1(0, 1)	-	0(0, 0)	0	A	[57015]
	33625.62	(0.03)	2(1, 2)	-	1(1, 1)	0	A	[57015]
	33626.01	(0.03)	2(1, 2)	-	1(1, 1)	0	E	[57015]

TABLE 13.6. Microwave spectrum of propylene — Continued

C₃H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	v_1	Sym.	Ref.
	34793.13	(0.03)	2(0, 2) - 1(0, 1)	0	E	[57015]
	34793.38	(0.03)	2(0, 2) - 1(0, 1)	0	A	[57015]
	36019.03	(0.03)	2(1, 1) - 1(1, 0)	0	E	[57015]
	36019.84	(0.03)	2(1, 1) - 1(1, 0)	0	A	[57015]
CH ₂ CH ¹³ CH ₃	32847.20	(0.10)	2(1, 2) - 1(1, 1)	0	A	[61013]
	33937.14	(0.10)	2(0, 2) - 1(0, 1)	0	A	[61013]
	35076.09	(0.10)	2(1, 1) - 1(1, 0)	0	E	[61013]
	35077.02	(0.10)	2(1, 1) - 1(1, 0)	0	A	[61013]
c-CHDCHCH ₃	32229.17	(0.05)	2(1, 2) - 1(1, 1)	0	A	[61013]
	33499.06	(0.05)	2(0, 2) - 1(0, 1)	0	A	[61013]
	34849.69	(0.05)	2(1, 1) - 1(1, 0)	0	E	[61013]
t-CHDCHCH ₃	6082.05	(0.20)	1(0, 1) - 0(0, 0)	1	A	[66045]
	16085.73	(0.20)	1(0, 1) - 0(0, 0)	1	E	[66045]
	16090.177	(0.200)	1(0, 1) - 0(0, 0)	0	A,E	[66045]
	31174.65	(0.20)	2(1, 2) - 1(1, 1)	0	A	[66045]
	31175.24	(0.20)	2(1, 2) - 1(1, 1)	0	E	[66045]
	31175.25	(0.20)	2(1, 2) - 1(1, 1)	1	A	[66045]
	31547.55	(0.20)	2(1, 2) - 1(1, 1)	1	E	[66045]
	32144.41	(0.20)	2(0, 2) - 1(0, 1)	1	A	[66045]
	32151.89	(0.20)	2(0, 2) - 1(0, 1)	1	E	[66045]
	32160.32	(0.20)	2(0, 2) - 1(0, 1)	0	A	[66045]
	32160.32	(0.20)	2(0, 2) - 1(0, 1)	0	E	[66045]
	32796.00	(0.20)	2(1, 1) - 1(1, 0)	1	E	[66045]
	33154.44	(0.20)	2(1, 1) - 1(1, 0)	1	A	[66045]
	33185.491	(0.200)	2(1, 1) - 1(1, 0)	0	E	[66045]
	33186.386	(0.200)	2(1, 1) - 1(1, 0)	0	A	[66045]
CH ₂ CDCH ₃	17128.02	(0.20)	1(0, 1) - 0(0, 0)	1	A	[66045]
	17131.31	(0.20)	1(0, 1) - 0(0, 0)	1	E	[66045]
	17138.997	(0.200)	1(0, 1) - 0(0, 0)	0	A,E	[66045]
	32807.79	(0.20)	2(1, 2) - 1(1, 1)	1	E	[66045]
	32813.399	(0.200)	2(1, 2) - 1(1, 1)	0	A	[66045]
	32813.453	(0.200)	2(1, 2) - 1(1, 1)	0	E	[66045]
	32985.41	(0.20)	2(1, 2) - 1(1, 1)	1	E	[66045]
	34202.14	(0.20)	2(0, 2) - 1(0, 1)	1	A	[66045]
	34209.03	(0.20)	2(0, 2) - 1(0, 1)	1	E	[66045]
	34223.637	(0.200)	2(0, 2) - 1(0, 1)	0	A	[66045]
	35540.31	(0.20)	2(1, 1) - 1(1, 0)	1	E	[66045]
	35705.11	(0.20)	2(1, 1) - 1(1, 0)	1	A	[66045]
	35742.374	(0.200)	2(1, 1) - 1(1, 0)	0	E	[66045]
	35742.775	(0.200)	2(1, 1) - 1(1, 0)	0	A	[66045]
sym-CH ₂ CHCH ₂ D	16832.90	(0.15)	1(0, 1) - 0(0, 0)	0		[58009]
	32364.93	(0.05)	2(1, 2) - 1(1, 1)	0	A	[61013]
	33626.41	(0.05)	2(0, 2) - 1(0, 1)	0	A	[61013]
	34966.94	(0.05)	2(1, 1) - 1(1, 0)	0	A	[61013]
asy-CH ₂ CHCH ₂ D	8370.50	(0.05)	17(3, 14) - 17(3, 15)	0		[68047]
	8831.43	(0.05)	10(2, 8) - 10(2, 9)	0		[68047]
	9407.14	(0.05)	4(1, 3) - 4(1, 4)	0		[68047]
	11444.67	(0.05)	18(3, 15) - 18(3, 16)	0		[68047]
	12481.33	(0.05)	11(2, 9) - 11(2, 10)	0		[68047]
	14106.06	(0.05)	5(1, 4) - 5(1, 5)	0		[68047]
	16377.116	(0.100)	1(0, 1) - 0(0, 0)	0		[70066]
	16379.54	(0.05)	1(0, 1) - 0(0, 0)	1	E	[70066]
	16379.99	(0.05)	1(0, 1) - 0(0, 0)	1	A	[70066]
	17018.66	(0.05)	12(2, 10) - 12(2, 11)	0		[68047]
	19737.07	(0.05)	6(1, 5) - 6(1, 6)	0		[68047]
	22500.50	(0.05)	13(2, 11) - 13(2, 12)	0		[68047]
	26291.77	(0.05)	7(1, 6) - 7(1, 7)	0		[68047]
	28961.55	(0.05)	14(2, 12) - 14(2, 13)	0		[68047]
	31399.682	(0.050)	2(1, 2) - 1(1, 1)	1	E-A	[68047]
	31813.36	(0.05)	2(1, 2) - 1(1, 1)	0	A	[61013]
	31852.17	(0.05)	2(1, 2) - 1(1, 1)	1	A	[68047]
	31953.879	(0.05)	2(1, 2) - 1(1, 1)	1	E	[68047]
	32735.34	(0.05)	2(0, 2) - 1(0, 1)	0	A	[61013]
	32740.49	(0.05)	2(0, 2) - 1(0, 1)	1	E	[70066]
	32741.51	(0.05)	2(0, 2) - 1(0, 1)	1	A	[70066]
	33565.347	(0.050)	2(1, 1) - 1(1, 0)	1	A	[68047]
	33667.14	(0.05)	2(1, 1) - 1(1, 0)	1	E	[68047]

TABLE 13.6. Microwave spectrum of propylene — Continued

C₃H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_1	Sym.	Ref.
	33695.17	(0.05)	2(1, 1) - 1(1, 0)	0	A	[61013]
	34119.667	(0.05)	3(1, 3) - 2(1, 2)	1	A-E	[68047]
	47744.37	(0.05)	3(1, 3) - 2(1, 2)	1	A	[68047]
	47751.57	(0.05)	3(1, 3) - 2(1, 2)	1	E	[68047]
	49055.60	(0.10)	3(0, 3) - 2(0, 2)	0		[70066]
	49064.24	(0.05)	3(0, 3) - 2(0, 2)	1	E	[70066]
	49066.05	(0.05)	3(0, 3) - 2(0, 2)	1	A	[70066]
	49133.40	(0.10)	3(2, 2) - 2(1, 1)	0	A	[70066]
	49135.28	(0.10)	3(2, 2) - 2(1, 1)	0	E	[70066]
	49163.01	(0.05)	3(2, 2) - 2(2, 1)	1	A	[70066]
	49169.39	(0.05)	3(2, 2) - 2(2, 1)	1	E	[70066]
	49191.66	(0.05)	3(2, 1) - 2(2, 0)	1	A	[70066]
	49196.04	(0.05)	3(2, 1) - 2(2, 0)	1	E	[70066]
	49202.95	(0.10)	3(2, 1) - 2(2, 0)	0	A	[70066]
	49204.77	(0.10)	3(2, 1) - 2(2, 0)	0	E	[70066]
	50503.25	(0.05)	3(1, 2) - 2(1, 1)	1	A	[68047]
	50510.57	(0.05)	3(1, 2) - 2(1, 1)	1	E	[68047]

Table 13.1A. Molecular constants for cyclopropane-1,1-d₂. [87019]

Parameter	$\text{CD}_2\text{CH}_2\text{CH}_2$	$\text{CH}_2\text{CH}_2\text{CH}_2^a$	$\text{CD}_2\text{CD}_2\text{CD}_2^b$
A (MHz)	18835.662(18)		
B (MHz)	16370.2703(70)	20093.317(30)	13832.06(60)
C (MHz)	11409.2285(67)	12522.3(90)	
Δ_J (MHz)	0.011246(12)	0.028985(29)	0.01148(51)
Δ_{JK} (MHz)	0.005087(35)	-0.037447(87)	
Δ_K (MHz)	0.00706(12)		
δ_J (MHz)	0.0030280(79)		
δ_K (MHz)	0.005561(27)		

^aJ. Pliva and J.W.C. Johns, Can. J. Phys. **62**, 1369 (1984).^bA.H. Nielsen, S.J. Daunt, and G.W. Halsey, J. Mol. Spectrosc. **81**, 494 (1980).

TABLE 13.2A. Microwave spectrum of cyclopropane

C₃H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
CD ₂ CH ₂ CH ₂	321268.010	(0.030)	11(5, 6) - 10(5, 5)	[87019]
	321824.834	(0.030)	11(10, 2) - 10(10, 1)	[87019]
D ₂ C-CH ₂ ∨ CH ₂	321844.590	(0.030)	11(10, 1) - 10(10, 0)	[87019]
	323955.440	(0.030)	11(9, 3) - 10(9, 2)	[87019]
	324386.186	(0.030)	11(9, 2) - 10(9, 1)	[87019]
	324408.298	(0.030)	11(7, 5) - 10(7, 4)	[87019]
	325467.300	(0.030)	14(0,14) - 13(0,13)	[87019]
	325842.859	(0.030)	11(8, 4) - 10(8, 3)	[87019]
	326946.663	(0.030)	13(2,11) - 12(2,10)	[87019]
	328659.275	(0.030)	12(5, 8) - 11(5, 7)	[87019]
	328767.649	(0.030)	12(4, 8) - 11(4, 7)	[87019]
	330013.656	(0.030)	11(8, 3) - 10(8, 2)	[87019]
	336505.346	(0.030)	11(6, 5) - 10(6, 4)	[87019]
	337600.932	(0.030)	14(1,13) - 13(1,12)	[87019]
	338682.422	(0.030)	11(7, 4) - 10(7, 3)	[87019]
	339135.753	(0.030)	13(4,10) - 12(4, 9)	[87019]
	339136.662	(0.030)	13(3,10) - 12(3, 9)	[87019]
	340804.130	(0.030)	12(6, 7) - 11(6, 6)	[87019]
	342197.491	(0.030)	12(5, 7) - 11(5, 6)	[87019]
	348271.963	(0.030)	15(0,15) - 14(0,14)	[87019]
	349745.818	(0.030)	14(2,12) - 13(2,11)	[87019]
	350881.725	(0.030)	12(11, 2) - 11(11, 1)	[87019]
	350888.518	(0.030)	12(11, 1) - 11(11, 0)	[87019]
	350945.579	(0.030)	12(7, 6) - 11(7, 5)	[87019]
	351413.027	(0.030)	13(5, 9) - 12(5, 8)	[87019]
	351435.011	(0.030)	13(4, 9) - 12(4, 8)	[87019]
	352996.924	(0.030)	12(10, 3) - 11(10, 2)	[87019]
	353169.261	(0.030)	12(10, 2) - 11(10, 1)	[87019]
	355390.625	(0.030)	12(9, 4) - 11(9, 3)	[87019]
	355847.597	(0.030)	12(8, 5) - 11(8, 4)	[87019]
	357507.248	(0.030)	12(9, 3) - 11(9, 2)	[87019]
	358790.477	(0.030)	12(6, 6) - 11(6, 5)	[87019]
	360403.585	(0.030)	15(1,14) - 14(1,13)	[87019]
	361920.815	(0.030)	14(3,11) - 13(3,10)	[87019]
	363784.137	(0.030)	13(6, 8) - 12(6, 7)	[87019]
364154.077	(0.030)	13(5, 8) - 12(5, 7)	[87019]	
366543.349	(0.030)	12(8, 4) - 11(8, 3)	[87019]	
370423.613	(0.030)	12(7, 5) - 11(7, 4)	[87019]	
371074.679	(0.030)	16(0,16) - 15(0,15)	[87019]	
372544.191	(0.030)	15(2,13) - 14(2,12)	[87019]	
374164.417	(0.030)	14(5,10) - 13(5, 9)	[87019]	
374168.480	(0.030)	14(4,10) - 13(4, 9)	[87019]	
375534.238	(0.030)	13(7, 7) - 12(7, 6)	[87019]	
378920.091	(0.030)	13(6, 7) - 12(6, 6)	[87019]	
379936.740	(0.030)	13(12, 2) - 12(12, 1)	[87019]	
379939.033	(0.030)	13(12, 1) - 12(12, 0)	[87019]	
381999.699	(0.030)	13(11, 3) - 12(11, 2)	[87019]	
382065.669	(0.030)	13(11, 2) - 12(11, 1)	[87019]	
383204.412	(0.030)	16(1,15) - 15(1,14)	[87019]	
383923.248	(0.030)	13(8, 6) - 12(8, 5)	[87019]	
384583.308	(0.030)	13(10, 4) - 12(10, 3)	[87019]	
384708.388	(0.030)	15(3,12) - 14(3,11)	[87019]	
385559.722	(0.030)	13(10, 3) - 12(10, 2)	[87019]	
386375.036	(0.030)	13(9, 5) - 12(9, 4)	[87019]	
386621.154	(0.030)	14(5, 9) - 13(5, 8)	[87019]	
386536.245	(0.030)	14(6, 9) - 13(6, 8)	[87019]	
393257.856	(0.030)	13(9, 4) - 12(9, 3)	[87019]	
393875.397	(0.030)	17(0,17) - 16(0,16)	[87019]	
395341.296	(0.030)	16(2,14) - 15(2,13)	[87019]	
395958.747	(0.030)	13(7, 6) - 12(7, 5)	[87019]	
396925.153	(0.030)	15(5,11) - 14(5,10)	[87019]	
396925.937	(0.030)	15(4,11) - 14(4,10)	[87019]	
398894.664	(0.030)	14(7, 8) - 13(7, 7)	[87019]	
399965.905	(0.030)	14(6, 8) - 13(6, 7)	[87019]	

Table 14.1. Molecular constants for propane.

Parameter	Ground State	$v_n=1_1$ State	$v_n=1_2$ State
<u>Rotational Constants</u>			
	[85022]	[67033]	[67033]
A (MHz)	29207.4815(31)	29166.55	29088.18
B (MHz)	8445.96770(71)	8432.45	8415.31
C (MHz)	7459.00196(73)	7449.47	7445.81
Δ_J (kHz)	7.19296(86)		
Δ_{JK} (kHz)	-26.9670(83)		
Δ_K (kHz)	159.845(94)		
δ_J (kHz)	1.39693(42)		
δ_K (kHz)	3.0585(75)		
ϕ_{JK} (Hz)	0.0296(101)		
ϕ_{KJ} (Hz)	-1.423(168)		
ϕ_K (Hz)	5.52(92)		
ϕ_J (Hz)	0.00368(28)		
<u>Internal Rotation Constants</u>			
	[85023]	[73084]	
ω_1 (s)	$-0.1909(29)10^{-5}$		
θ_a	35.17(64)		
θ_b	54.83(64)	57.07	
I_α (u Å ²)	3.198(21)	3.13	
s	80.22(15)	80.10(25)	
F (GHz)	183.99(121)	191.64	
V_3 (cm ⁻¹)	1108.(10)	1153.(4)	
$V_{1_2}^1$ (cm ⁻¹)		-51.8(8)	
<u>Electric Dipole Moment</u> [66042]			
μ_b (D)	0.0848(10) ^a		

^aAverage of values for several transitions.

Table 14.2. Rotational constants and electric dipole moment for ^{13}C and deuterated isotopic species of propane.

Isotopic Species	A (MHz)	B (MHz)	C (MHz)
<u>Rotational Constants</u> [60009]			
$^{13}\text{CH}_3\text{CH}_2\text{CH}_3$	29092.05(10)	8228.77(10)	7281.73(10)
$\text{CH}_3\text{ }^{13}\text{CH}_2\text{CH}_3$	28660.90(10)	8447.11(10)	7423.19(10)
$\text{CH}_3\text{CHDCH}_3$	25829.94(10)	8358.76(10)	7283.00(10)
sym- $\text{CH}_2\text{DCH}_2\text{CH}_3$	29017.79(10)	7838.32(10)	6971.96(10)
asy- $\text{CH}_2\text{DCH}_2\text{CH}_3$	26828.97(10)	8123.10(10)	7185.14(10)
<u>Electric Dipole Moment</u> [66042]			
$\text{CH}_3\text{CD}_2\text{CH}_3$	$\mu_{\text{D}} = 0.095(1)^{\text{a}}$ D		
$\text{CD}_3\text{CH}_2\text{CD}_3$	$\mu_{\text{D}} = 0.076(1)^{\text{a}}$ D		

^aAverage of values for several transitions.

TABLE 14.3. Microwave spectrum of propane

C₃H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	$\nu_1 \nu_2$	Sym.	Ref.
CH ₃ CH ₂ CH ₃	8308.032	(0.030)	7(2, 5)	- 6(3, 4)	AA	[85023]
	8308.279	(0.030)	7(2, 5)	- 6(3, 4)	EE	[85023]
	8308.534	(0.030)	7(2, 5)	- 6(3, 4)	AE+EA	[85023]
	8877.344	(0.020)	29(12,18)	- 30(11,19)		[85022]
	8954.121	(0.030)	5(3, 3)	- 6(2, 4)	EA	[85023]
	8954.195	(0.030)	5(3, 3)	- 6(2, 4)	AE	[85023]
	8954.414	(0.030)	5(3, 3)	- 6(2, 4)	EE	[85023]
	8954.680	(0.030)	5(3, 3)	- 6(2, 4)	AA	[85023]
	9281.940	(0.030)	21(9,13)	- 22(8,14)	AE	[85023]
	9282.033	(0.030)	21(9,12)	- 22(8,15)	*EE	[85023]
	9282.238	(0.030)	21(9,13)	- 22(8,14)	AA	[85023]
	9282.328	(0.030)	21(9,12)	- 22(8,15)	AA	[85023]
	9723.963	(0.030)	13(6, 8)	- 14(5, 9)	EA	[85023]
	9724.884	(0.030)	13(6, 8)	- 14(5, 9)	EE	[85023]
	9725.085	(0.030)	13(6, 8)	- 14(5, 9)	AE	[85022]
	9725.680	(0.030)	13(6, 8)	- 14(5, 9)	AA	[85023]
	9725.982	(0.030)	13(6, 7)	- 14(5,10)	*EE	[85023]
	9744.810	(0.030)	13(6, 8)	- 14(5, 9)	*EE	[85023]
	9745.145	(0.030)	13(6, 7)	- 14(5,10)	AE	[85023]
	9745.720	(0.030)	13(6, 7)	- 14(5,10)	AA	[85023]
	9745.910	(0.030)	13(6, 7)	- 14(5,10)	EE	[85023]
	9746.203	(0.030)	13(6, 7)	- 14(5,10)	*EA	[85023]
	11013.883	(0.030)	2(0, 2)	- 1(1, 1)	AA	[85023]
	11013.937	(0.030)	2(0, 2)	- 1(1, 1)	EE	[85023]
	11013.995	(0.030)	2(0, 2)	- 1(1, 1)	AE	[85023]
	11014.005	(0.030)	2(0, 2)	- 1(1, 1)	EA	[85023]
	11124.522	(0.030)	10(3, 8)	- 9(4, 5)	AA	[85023]
	11124.784	(0.030)	10(3, 8)	- 9(4, 5)	EE	[85023]
	11125.007	(0.030)	10(3, 8)	- 9(4, 5)	EA	[85023]
	11319.739	(0.030)	5(3, 2)	- 6(2, 5)	AE	[85023]
	11319.824	(0.030)	5(3, 2)	- 6(2, 5)	EA	[85023]
	11320.043	(0.030)	5(3, 2)	- 6(2, 5)	EE	[85023]
	11320.299	(0.030)	5(3, 2)	- 6(2, 5)	AA	[85023]
	12061.159	(0.030)	18(6,13)	- 17(7,10)	EA	[85023]
	12061.408	(0.030)	18(6,13)	- 17(7,10)	EE	[85023]
	12061.542	(0.030)	18(6,13)	- 17(7,10)	AA	[85023]
	12062.003	(0.030)	18(6,13)	- 17(7,10)	AE	[85023]
	12062.204	(0.030)	18(6,12)	- 17(7,11)	*EE	[85023]
	12070.246	(0.030)	18(6,13)	- 17(7,10)	*EE	[85023]
	12070.427	(0.030)	18(6,12)	- 17(7,11)	AA	[85023]
	12070.912	(0.030)	18(6,12)	- 17(7,11)	AE	[85023]
	12071.045	(0.030)	18(6,12)	- 17(7,11)	EE	[85023]
	12071.742	(0.030)	18(6,12)	- 17(7,11)	EA	[85023]
	12381.595	(0.030)	10(3, 7)	- 9(4, 6)	AA	[85023]
	12381.901	(0.030)	10(3, 7)	- 9(4, 6)	EE	[85023]
	12382.165	(0.030)	10(3, 7)	- 9(4, 6)	AE	[85023]
	12382.264	(0.030)	10(3, 7)	- 9(4, 6)	EA	[85023]
	12435.726	(0.020)	26(9,18)	- 25(10,15)		[85022]
	12435.726	(0.020)	26(9,17)	- 25(10,16)		[85022]
	14384.156	(0.020)	26(11,15)	- 27(10,18)		[85022]
	14824.451	(0.030)	18(8,11)	- 19(7,12)	AE	[85023]
	14824.742	(0.030)	18(8,10)	- 19(7,13)	*EE	[85023]
	14824.870	(0.030)	18(8,11)	- 19(7,12)	AA	[85023]
	14824.910	(0.030)	18(8,10)	- 19(7,13)	AE	[85023]
14825.049	(0.030)	18(8,11)	- 19(7,12)	*EE	[85023]	
14825.331	(0.030)	18(8,10)	- 19(7,13)	AA	[85023]	
15245.380	(0.030)	10(5, 6)	- 11(4, 7)	EA	[85023]	
15246.273	(0.030)	10(5, 6)	- 11(4, 7)	EE	[85023]	
15246.963	(0.030)	10(5, 6)	- 11(4, 7)	AA	[85023]	
15247.652	(0.030)	10(5, 5)	- 11(4, 8)	*EE	[85023]	
15247.888	(0.030)	10(5, 5)	- 11(4, 8)	*EA	[85023]	
15330.706	(0.030)	10(5, 6)	- 11(4, 7)	*EA	[85023]	
15331.599	(0.030)	10(5, 6)	- 11(4, 7)	*EE	[85023]	
15332.312	(0.030)	10(5, 5)	- 11(4, 8)	AE	[85023]	
15332.930	(0.030)	10(5, 5)	- 11(4, 8)	AA	[85023]	
15332.998	(0.030)	10(5, 5)	- 11(4, 8)	EE	[85023]	
15333.286	(0.030)	10(5, 5)	- 11(4, 8)	EA	[85023]	
17119.125	(0.030)	13(4,10)	- 12(5, 7)	AA	[85023]	

TABLE 14.3. Microwave spectrum of propane — Continued

C₃H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	$\nu_1 \nu_2$	Sym.	Ref.
	17119.340	(0.030)	13(4,10) - 12(5, 7)		EE	[85023]
	17119.436	(0.030)	13(4,10) - 12(5, 7)		EA	[85023]
	17119.736	(0.030)	13(4,10) - 12(5, 7)		AE	[85023]
	17440.628	(0.030)	13(4, 9) - 12(5, 8)		AA	[85023]
	17441.010	(0.030)	13(4, 9) - 12(5, 8)		EE	[85023]
	17441.253	(0.030)	13(4, 9) - 12(5, 8)		AE	[85023]
	17441.521	(0.030)	13(4, 9) - 12(5, 8)		EA	[85023]
	17611.181	(0.030)	21(7,15) - 20(8,12)		EE	[85023]
	17611.284	(0.030)	21(7,15) - 20(8,12)		AA	[85023]
	17612.676	(0.030)	21(7,14) - 20(8,13)		*EE	[85023]
	17613.194	(0.030)	21(7,14) - 20(8,13)		AA	[85023]
	17613.698	(0.030)	21(7,14) - 20(8,13)		EE	[85023]
	19250.538	(0.030)	8(2, 7) - 7(3, 4)		AA	[85023]
	19250.766	(0.030)	8(2, 7) - 7(3, 4)		EE	[85023]
	19250.992	(0.030)	8(2, 7) - 7(3, 4)		AE	[85023]
	20371.965	(0.030)	15(7, 9) - 16(6,10)		AE	[85023]
	20371.990	(0.030)	15(7, 9) - 16(6,10)		EE	[85023]
	20372.790	(0.030)	15(7, 9) - 16(6,10)		AA	[85023]
	20372.864	(0.030)	15(7, 8) - 16(6,11)		*EE	[85023]
	20374.330	(0.030)	15(7, 9) - 16(6,10)		*EE	[85023]
	20374.404	(0.030)	15(7, 8) - 16(6,11)		AE	[85023]
	20374.951	(0.030)	15(7, 8) - 16(6,11)		AA	[85023]
	20375.202	(0.030)	15(7, 8) - 16(6,11)		EE	[85023]
	20657.876	(0.030)	7(4, 4) - 8(3, 5)		EA	[85022]
	20658.414	(0.030)	7(4, 4) - 8(3, 5)		AE	[85022]
	20658.573	(0.030)	7(4, 4) - 8(3, 5)		EE	[85022]
	20659.021	(0.030)	7(4, 4) - 8(3, 5)		AA	[85022]
	21001.174	(0.030)	7(4, 3) - 8(3, 6)		AE	[85023]
	21001.615	(0.030)	7(4, 3) - 8(3, 6)		EE	[85023]
	21001.786	(0.030)	7(4, 3) - 8(3, 6)		AA	[85023]
	21642.31	(0.05)	1(1, 0) - 1(0, 1)	1 2	A ₂ A ₁	[73084]
	21644.27	(0.05)	1(1, 0) - 1(0, 1)	1 2	EE	[73084]
	21646.21	(0.05)	1(1, 0) - 1(0, 1)	1 2	A ₂ E	[73084]
	21646.21	(0.05)	1(1, 0) - 1(0, 1)	1 2	EA ₁	[73084]
	21717.05	(0.05)	1(1, 0) - 1(0, 1)	1 1	A ₁ A ₂	[73084]
	21718.67	(0.05)	1(1, 0) - 1(0, 1)	1 1	EE	[73084]
	21720.33	(0.05)	1(1, 0) - 1(0, 1)	1 1	A ₁ E	[73084]
	21720.33	(0.05)	1(1, 0) - 1(0, 1)	1 1	EA ₂	[73084]
	21748.288	(0.030)	1(1, 0) - 1(0, 1)		AE + EA	[85023]
	21748.363	(0.030)	1(1, 0) - 1(0, 1)		EE	[85023]
	21748.432	(0.030)	1(1, 0) - 1(0, 1)		AA	[85023]
	22645.06	(0.05)	2(1, 1) - 2(0, 2)	1 2	A ₂ A ₁	[73048]
	22647.00	(0.05)	2(1, 1) - 2(0, 2)	1 2	EE	[73048]
	22648.99	(0.05)	2(1, 1) - 2(0, 2)	1 2	A ₂ E	[73048]
	22648.99	(0.05)	2(1, 1) - 2(0, 2)	1 2	E ₁	[73048]
	22733.90	(0.05)	2(1, 1) - 2(0, 2)	1 1	A ₁ A ₂	[73048]
	22735.68	(0.05)	2(1, 1) - 2(0, 2)	1 1	EE	[73048]
	22737.35	(0.05)	2(1, 1) - 2(0, 2)	1 1	A ₁ E	[73048]
	22737.35	(0.05)	2(1, 1) - 2(0, 2)	1 1	EA ₂	[73048]
	22769.662	(0.030)	2(1, 1) - 2(0, 2)		AE + EA	[85023]
	22769.737	(0.030)	2(1, 1) - 2(0, 2)		EE	[85023]
	22769.813	(0.030)	2(1, 1) - 2(0, 2)		AA	[85023]
	22786.123	(0.030)	16(5,12) - 15(6, 9)		AA	[85023]
	22786.199	(0.030)	16(5,12) - 15(6, 9)		EE	[85023]
	22786.695	(0.030)	16(5,12) - 15(6, 9)		AE	[85023]
	22861.950	(0.030)	16(5,11) - 15(6,10)		AA	[85023]
	22862.444	(0.030)	16(5,11) - 15(6,10)		EE	[85023]
	22862.528	(0.030)	16(5,11) - 15(6,10)		AE	[85023]
	22933.680	(0.030)	5(1, 4) - 4(2, 3)		AA	[85022]
	22933.830	(0.030)	5(1, 4) - 4(2, 3)		EE	[85022]
	22933.985	(0.030)	5(1, 4) - 4(2, 3)		AE + EA	[85022]
	24210.73	(0.05)	3(1, 2) - 3(0, 3)	1 2	A ₂ A ₁	[73048]
	24212.82	(0.05)	3(1, 2) - 3(0, 3)	1 2	EE	[73048]
	24214.99	(0.05)	3(1, 2) - 3(0, 3)	1 2	A ₂ E	[73048]
	24214.99	(0.05)	3(1, 2) - 3(0, 3)	1 2	EA ₁	[73048]
	24322.78	(0.05)	3(1, 2) - 3(0, 3)	1 1	A ₁ A ₂	[73048]
	24324.54	(0.05)	3(1, 2) - 3(0, 3)	1 1	EE	[73048]

TABLE 14.3. Microwave spectrum of propane — Continued

C₃H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	$\nu_1 \nu_2$	Sym.	Ref.
	24326.37	(0.05)	3(1, 2) - 3(0, 3)	1 1	A ₁ E	[73048]
	24326.37	(0.05)	3(1, 2) - 3(0, 3)	1 1	EA ₂	[73048]
	24365.370	(0.030)	3(1, 2) - 3(0, 3)		AE + EA	[85023]
	24365.451	(0.030)	3(1, 2) - 3(0, 3)		EE	[85023]
	24365.531	(0.030)	3(1, 2) - 3(0, 3)		AA	[85023]
	25916.034	(0.030)	12(6, 7) - 13(5, 8)		EE	[85023]
	25916.258	(0.030)	12(6, 7) - 13(5, 8)		AE	[85023]
	25916.931	(0.030)	12(6, 7) - 13(5, 8)		AA	[85023]
	25917.154	(0.030)	12(6, 6) - 13(5, 9)		EE	[85023]
	25925.572	(0.030)	12(6, 7) - 13(5, 8)		EE	[85023]
	25925.804	(0.030)	12(6, 6) - 13(5, 9)		AE	[85023]
	25926.705	(0.030)	12(6, 6) - 13(5, 9)		EE	[85023]
	25926.452	(0.030)	12(6, 6) - 13(5, 9)		AA	[85023]
	26132.816	(0.030)	8(2, 6) - 7(3, 5)		AA	[85023]
	26133.035	(0.030)	8(2, 6) - 7(3, 5)		EE	[85023]
	26133.245	(0.030)	8(2, 6) - 7(3, 5)		AE + EA	[85023]
	26411.06	(0.05)	4(1, 3) - 4(0, 4)	1 2	A ₂ A ₁	[73048]
	26413.30	(0.05)	4(1, 3) - 4(0, 4)	1 2	EE	[73048]
	26415.55	(0.05)	4(1, 3) - 4(0, 4)	1 2	A ₂ E	[73048]
	26415.55	(0.05)	4(1, 3) - 4(0, 4)	1 2	EA ₁	[73048]
	26556.51	(0.05)	4(1, 3) - 4(0, 4)	1 1	A ₁ A ₂	[73048]
	26558.40	(0.05)	4(1, 3) - 4(0, 4)	1 1	EE	[73048]
	26560.30	(0.05)	4(1, 3) - 4(0, 4)	1 1	A ₁ E	[73048]
	26560.30	(0.05)	4(1, 3) - 4(0, 4)	1 1	EA ₂	[73048]
	26609.24	(0.03)	4(1, 3) - 4(0, 4)			[60009]
	29334.72	(0.05)	5(1, 4) - 5(0, 5)	1 2	A ₂ A ₁	[67033]
	29337.18	(0.05)	5(1, 4) - 5(0, 5)	1 2	EE	[67033]
	29339.60	(0.05)	5(1, 4) - 5(0, 5)	1 2	A ₂ E	[67033]
	29339.60	(0.05)	5(1, 4) - 5(0, 5)	1 2	EA ₁	[67033]
	29525.87	(0.05)	5(1, 4) - 5(0, 5)	1 1	A ₁ A ₂	[67033]
	29527.91	(0.05)	5(1, 4) - 5(0, 5)	1 1	EE	[67033]
	29529.98	(0.05)	5(1, 4) - 5(0, 5)	1 1	A ₁ E	[67033]
	29529.98	(0.05)	5(1, 4) - 5(0, 5)	1 1	EA ₂	[67033]
	29592.51	(0.03)	5(1, 4) - 5(0, 5)			[60009]
	33414.72	(0.03)	6(1, 5) - 6(0, 6)			[60009]
	36616.05	(0.05)	1(1, 1) - 0(0, 0)	1 1	A ₁ A ₂	[73084]
	36617.73	(0.05)	1(1, 1) - 0(0, 0)	1 1	EE	[73084]
	36619.24	(0.05)	1(1, 1) - 0(0, 0)	1 1	A ₁ E	[73084]
	36619.24	(0.05)	1(1, 1) - 0(0, 0)	1 1	EA ₂	[73084]
	36534.10	(0.05)	1(1, 1) - 0(0, 0)	1 2	A ₂ A ₁	[73084]
	36535.95	(0.05)	1(1, 1) - 0(0, 0)	1 2	EE	[73084]
	36537.80	(0.05)	1(1, 1) - 0(0, 0)	1 2	A ₂ E	[73084]
	36537.80	(0.05)	1(1, 1) - 0(0, 0)	1 2	EA ₁	[73084]
	36666.33	(0.05)	1(1, 1) - 0(0, 0)			[60009]
	51425.55	(0.05)	2(1, 2) - 1(0, 1)	1 2	A ₂ A ₁	[73084]
	51427.45	(0.05)	2(1, 2) - 1(0, 1)	1 2	EE	[73084]
	51429.25	(0.05)	2(1, 2) - 1(0, 1)	1 2	A ₂ E	[73084]
	51429.25	(0.05)	2(1, 2) - 1(0, 1)	1 2	EA ₁	[73084]
	51514.95	(0.05)	2(1, 2) - 1(0, 1)	1 1	A ₁ A ₂	[73084]
	51516.55	(0.05)	2(1, 2) - 1(0, 1)	1 1	EE	[73084]
	51518.15	(0.05)	2(1, 2) - 1(0, 1)	1 1	A ₁ E	[73084]
	51518.15	(0.05)	2(1, 2) - 1(0, 1)	1 1	EA ₂	[73084]
	140017.440	(0.010)	18(1, 17) - 18(0, 18)			[15022]
	140209.001	(0.010)	29(5, 24) - 29(4, 25)			[85022]
	140620.619	(0.010)	17(2, 16) - 17(1, 17)			[85022]
	141025.107	(0.010)	36(5, 31) - 36(4, 32)			[85022]
	141203.180	(0.010)	14(4, 10) - 14(3, 11)			[85022]
	141387.150	(0.010)	27(3, 24) - 27(2, 25)			[85022]
	142672.637	(0.010)	17(3, 14) - 16(4, 13)			[85022]
	142955.170	(0.010)	32(4, 28) - 32(3, 29)			[85022]
	143346.340	(0.010)	13(4, 9) - 13(3, 10)			[85022]
	143622.180	(0.010)	19(3, 17) - 19(2, 18)			[85022]
	144760.500	(0.010)	28(5, 23) - 28(4, 24)			[85022]
	145001.150	(0.010)	12(4, 8) - 12(3, 9)			[85022]
	145856.220	(0.010)	19(3, 17) - 18(4, 14)			[85022]
	146021.260	(0.010)	14(2, 12) - 13(3, 11)			[85022]
	146232.500	(0.010)	11(4, 7) - 11(3, 8)			[85022]

MICROWAVE SPECTRAL TABLES

TABLE 14.3. Microwave spectrum of propane — Continued

C₃H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	$\nu_1 \nu_2$	Sym.	Ref.
	146232.500	(0.010)	11(4, 7)	- 11(3, 8)		[85022]
	146601.280	(0.010)	9(1, 9)	- 8(0, 8)		[85022]
	147044.370	(0.010)	21(4,18)	- 20(5,15)		[85022]
	147116.440	(0.010)	10(4, 6)	- 10(3, 7)		[85022]
	147362.080	(0.010)	37(5,32)	- 37(4,33)		[85022]
	147538.060	(0.010)	10(0,10)	- 9(1, 9)		[85022]
	147728.480	(0.010)	9(4, 5)	- 9(3, 6)		[85022]
	148136.610	(0.010)	8(4, 4)	- 8(3, 5)		[85022]
	211188.559	(0.010)	32(5,28)	- 32(4,29)		[85022]
	211446.958	(0.010)	14(0,14)	- 13(1,13)		[85022]
	211481.852	(0.010)	8(2, 6)	- 7(1, 7)		[85022]
	211766.984	(0.010)	17(2,15)	- 16(3,14)		[85022]
	212660.630	(0.010)	11(2,10)	- 10(1, 9)		[85022]
	212717.237	(0.010)	28(3,26)	- 28(2,27)		[85022]
	213455.847	(0.010)	28(6,22)	- 28(5,23)		[85022]
	214776.052	(0.010)	33(3,30)	- 33(2,31)		[85022]
	214833.358	(0.010)	31(4,28)	- 31(3,29)		[85022]
	215513.772	(0.010)	14(1,14)	- 13(0,13)		[85022]
	216107.921	(0.010)	27(5,22)	- 26(6,21)		[85022]
	216117.906	(0.010)	7(3, 5)	- 6(2, 4)		[85022]
	216255.769	(0.010)	33(5,29)	- 33(4,30)		[85022]
	217127.058	(0.010)	27(6,21)	- 27(5,22)		[85022]
	217297.294	(0.010)	15(1,14)	- 14(2,13)		[85022]
	218618.306	(0.010)	7(3, 4)	- 6(2, 5)		[85022]
	219527.413	(0.010)	26(1,25)	- 26(0,26)		[85022]
	220215.357	(0.010)	26(6,20)	- 26(5,21)		[85022]
	220436.493	(0.010)	26(2,25)	- 26(1,26)		[85022]
	221631.655	(0.010)	29(3,27)	- 29(2,28)		[85022]
	221857.648	(0.010)	34(5,30)	- 34(4,31)		[85022]
	280971.706	(0.010)	17(2,16)	- 16(1,15)		[85022]
	283543.557	(0.010)	12(3,10)	- 11(2, 9)		[85022]
	286689.990	(0.010)	6(5, 2)	- 5(4, 1)		[85022]
	287574.584	(0.010)	19(0,19)	- 18(1,18)		[85022]
	288181.882	(0.010)	11(3, 8)	- 10(2, 9)		[85022]
	288365.749	(0.010)	19(1,19)	- 18(0,18)		[85022]
	288605.341	(0.010)	41(8,33)	- 41(7,34)		[85022]
	289146.451	(0.010)	19(1,18)	- 18(2,17)		[85022]
	291586.293	(0.010)	9(4, 6)	- 8(3, 5)		[85022]
	291944.025	(0.010)	9(4, 5)	- 8(3, 6)		[85022]
	293185.436	(0.010)	18(2,17)	- 17(1,16)		[85022]
	293477.608	(0.010)	27(4,23)	- 26(5,22)		[85022]
	295099.457	(0.010)	13(3,11)	- 12(2,10)		[85022]
	296256.010	(0.010)	39(8,31)	- 39(7,32)		[85022]
¹³ CH ₃ CH ₂ CH ₃	22788.80	(0.06)	2(1, 1)	- 2(0, 2)		[60009]
	24315.01	(0.06)	3(1, 2)	- 3(0, 3)		[60009]
	26456.74	(0.06)	4(1, 3)	- 4(0, 4)		[60009]
	29298.58	(0.06)	5(1, 4)	- 5(0, 5)		[60009]
	32933.58	(0.06)	6(1, 5)	- 6(0, 6)		[60009]
	36373.78	(0.06)	1(1, 1)	- 0(0, 0)		[60009]
CH ₃ ¹³ CH ₂ CH ₃	22299.03	(0.06)	2(1, 1)	- 2(0, 2)		[60009]
	23961.76	(0.06)	3(1, 2)	- 3(0, 3)		[60009]
	26306.35	(0.06)	4(1, 3)	- 4(0, 4)		[60009]
	29432.48	(0.06)	5(1, 4)	- 5(0, 5)		[60009]
	33446.47	(0.06)	6(1, 5)	- 6(0, 6)		[60009]
	36083.69	(0.06)	1(1, 1)	- 0(0, 0)		[60009]
CH ₃ CHDCH ₃	19670.78	(0.06)	2(1, 1)	- 2(0, 2)		[60009]
	21445.48	(0.06)	3(1, 2)	- 3(0, 3)		[60009]
	23971.76	(0.06)	4(1, 3)	- 4(0, 4)		[60009]
	27370.09	(0.06)	5(1, 4)	- 5(0, 5)		[60009]
	31759.70	(0.06)	6(1, 5)	- 6(0, 6)		[60009]
	33112.93	(0.06)	1(1, 1)	- 0(0, 0)		[60009]
sym-CH ₂ DCH ₂ CH ₃	22938.16	(0.06)	2(1, 1)	- 2(0, 2)		[60009]
	24324.96	(0.06)	3(1, 2)	- 3(0, 3)		[60009]
	26262.62	(0.06)	4(1, 3)	- 4(0, 4)		[60009]
	28822.23	(0.06)	5(1, 4)	- 5(0, 5)		[60009]
	32083.91	(0.06)	6(1, 5)	- 6(0, 6)		[60009]
	35989.76	(0.06)	1(1, 1)	- 0(0, 0)		[60009]

TABLE 14.3. Microwave spectrum of propane — Continued

C₃H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$ $v_1 v_2$	Sym.	Ref.
<i>asy</i> -CH ₂ DCH ₂ CH ₃	20616.12	(0.06)	2(1, 1) - 2(0, 2)		[60009]
	22137.98	(0.06)	3(1, 2) - 3(0, 3)		[60009]
	24283.11	(0.06)	4(1, 3) - 4(0, 4)		[60009]
	27141.90	(0.06)	5(1, 4) - 5(0, 5)		[60009]
	30811.32	(0.06)	6(1, 5) - 6(0, 6)		[60009]
	34014.10	(0.06)	1(1, 1) - 0(0, 0)		[60009]

Table 15.1. Molecular constants for the C₄H radical.

Parameter	Ground State [83053]	v=1 State [87018]
B (MHz)	4758.6557(7)	4782.160(2)
D (kHz)	0.8627(10)	0.910(2)
γ (MHz)	-38.555(2)	-56.97(13)
γ _D (kHz)	0.127	1.40(9)
b (MHz)	-19.088(6)	
c (MHz)	12.435(10)	

TABLE 15.2. Microwave spectrum of butadiynyl radical

C₄H

Isotopic species	Frequency (MHz)	Unc. (MHz)	J' - J''	P	$F' - F''$	Vib. state	Ref.
C ₄ H	9493.067	(0.003)	3/2 - 1/2		1 - 0	$\nu = 0$	[83052]
	9497.624	(0.003)	3/2 - 1/2		2 - 1	$\nu = 0$	[83052]
	9508.016	(0.003)	3/2 - 1/2		1 - 1	$\nu = 0$	[83052]
	9547.967	(0.003)	1/2 - 1/2		1 - 0	$\nu = 0$	[83052]
	9551.728	(0.003)	1/2 - 1/2		0 - 1	$\nu = 0$	[83052]
	9562.915	(0.003)	1/2 - 1/2		1 - 1	$\nu = 0$	[83052]
	85633.9	(1.0)	19/2 - 17/2			$\nu = 0$	[78032]
	85672.4	(1.0)	17/2 - 15/2			$\nu = 0$	[78032]
	86048.50	(0.25)	9/1 - 8/1	<i>l</i>		$\nu = 1$	[87018]
	86104.44	(0.25)	9/1 - 8/1	<i>u</i>		$\nu = 1$	[87018]
	95149.5	(1.0)	21/2 - 19/2			$\nu = 0$	[78032]
	95189.0	(1.0)	19/2 - 17/2			$\nu = 0$	[78032]
	95611.13	(0.25)	10/1 - 9/1	<i>l</i>		$\nu = 1$	[87018]
	95667.89	(0.25)	10/1 - 9/1	<i>u</i>		$\nu = 1$	[87018]
	104667.3	(1.0)	23/2 - 21/2			$\nu = 0$	[78032]
	104706.0	(1.0)	21/2 - 19/2			$\nu = 0$	[78032]
	105174.58	(0.20)	11/1 - 10/1	<i>l</i>		$\nu = 1$	[87018]
	105230.65	(0.20)	11/1 - 10/1	<i>u</i>		$\nu = 1$	[87018]
	114182.	(1.0)	25/2 - 23/2			$\nu = 0$	[78032]
	114221.	(1.0)	23/2 - 21/2			$\nu = 0$	[78032]
	114737.17	(0.20)	12/1 - 11/1	<i>l</i>		$\nu = 1$	[87018]
	114793.82	(0.35)	12/1 - 11/1	<i>u</i>		$\nu = 1$	[87018]
	133862.50	(0.20)	14/1 - 13/1	<i>l</i>		$\nu = 1$	[87018]
	133918.54	(0.20)	14/1 - 13/1	<i>u</i>		$\nu = 1$	[87018]
	142728.773	(0.018)	31/2 - 29/2			$\nu = 0$	[83053]
	142767.280	(0.016)	29/2 - 27/2			$\nu = 0$	[83053]
	143424.39	(0.20)	15/1 - 14/1	<i>l</i>		$\nu = 1$	[87018]
	143480.41	(0.20)	15/1 - 14/1	<i>u</i>		$\nu = 1$	[87018]
	152986.00	(0.20)	16/1 - 15/1	<i>l</i>		$\nu = 1$	[87018]
	153041.88	(0.20)	16/1 - 15/1	<i>u</i>		$\nu = 1$	[87018]
	162547.41	(0.15)	17/1 - 16/1	<i>l</i>		$\nu = 1$	[87018]
	162603.18	(0.15)	17/1 - 16/1	<i>u</i>		$\nu = 1$	[87018]
	171272.249	(0.014)	37/2 - 35/2			$\nu = 0$	[83053]
	171310.707	(0.014)	35/2 - 33/2			$\nu = 0$	[83053]
	172108.36	(0.50)	18/1 - 17/1	<i>l</i>		$\nu = 1$	[87018]
	172164.12	(0.80)	18/1 - 17/1	<i>u</i>		$\nu = 1$	[87018]
	180786.031	(0.017)	39/2 - 37/2			$\nu = 0$	[83053]
	180824.472	(0.016)	37/2 - 35/2			$\nu = 0$	[83053]
	181669.38	(0.03)	19/1 - 18/1	<i>l</i>		$\nu = 1$	[87018]
	181725.00	(0.05)	19/1 - 18/1	<i>u</i>		$\nu = 1$	[87018]
	190299.425	(0.014)	41/2 - 39/2			$\nu = 0$	[83053]
	190337.804	(0.013)	39/2 - 37/2			$\nu = 0$	[83053]
	191229.68	(0.04)	20/1 - 19/1	<i>l</i>		$\nu = 1$	[87018]
	191285.01	(0.06)	20/1 - 19/1	<i>u</i>		$\nu = 1$	[87018]
	199812.391	(0.016)	43/2 - 41/2			$\nu = 0$	[83053]
	199850.787	(0.015)	41/2 - 39/2			$\nu = 0$	[83053]
	200789.44	(0.04)	21/1 - 20/1	<i>l</i>		$\nu = 1$	[87018]
	200844.62	(0.04)	21/1 - 20/1	<i>u</i>		$\nu = 1$	[87018]
	210348.87	(0.05)	22/1 - 21/1	<i>l</i>		$\nu = 1$	[87018]
	210403.74	(0.04)	22/1 - 21/1	<i>u</i>		$\nu = 1$	[87018]
	219907.70	(0.03)	23/1 - 22/1	<i>l</i>		$\nu = 1$	[87018]
	219962.41	(0.05)	23/1 - 22/1	<i>u</i>		$\nu = 1$	[87018]

Table 16.1. Molecular constants of 1,3-butadiyne (diacetylene) in excited vibrational states.

Parameter	Upper State ^a	Lower State ^a
<u>$\nu_8 - \nu_6$ band [81046]</u>		
	<u>ν_8</u>	<u>ν_6</u>
B_V (MHz)	4391.1921(94)	4391.3230(84)
D_V (kHz)	0.594(179)	0.582(154)
q_V (MHz)	2.4073(37)	2.4830(32)
ΔG_V (MHz)	71868.336(57)	
μ (D)	0.0787(10)	
<u>$\Sigma_g^+ - \Sigma_u^+$ subband [82036]</u>		
	<u>$\nu_8 + \nu_9$ (g)</u>	<u>$\nu_6 + \nu_9$ (u)</u>
B_V (MHz)	4402.9090(61)	4403.8625(56)
D_V (kHz)	0.854(54)	1.826(47)
H_V (Hz)	-0.118(155)	0.003(121)
ΔG_V (MHz)	46112.301(42)	
μ (D)	0.0755(5)	
<u>$\Sigma_g^- - \Sigma_u^-$ subband [82036]</u>		
B_V (MHz)	4403.7414(36)	4403.8795(41)
D_V (MHz)	0.713(37)	0.767(43)
H_V (Hz)	0.243(207)	0.212(179)
ΔG_V (MHz)	73412.284(29)	
μ (D)	0.0805(4)	
<u>$\Delta_g - \Delta_u$ subband [82036]</u>		
B_V (MHz)	4403.7192(56)	4403.8715(64)
D_V (kHz)	0.302(49)	-0.216(56)
H_V (Hz)	0.425(229)	0.296(201)
ρ_V (kHz)	0.0492(134)	0.5185(128)
ρ_V^\dagger (Hz)	0.320(68)	0.212(57)
ΔG_V (MHz)	77573.622(58)	

^aValues in parentheses denote 2.5 standard errors.

Table 16.2. Molecular constants of HC=CC=CD. [81047]

State	B (MHz)	D (kHz)	q (MHz)	μ (D)
ν_6 (Π)	4086.2165(44) ^a	0.408(36)	2.1316(28)	0.0907(6)
$2\nu_6$ (Δ)	4087.6963(58)	0.349(50)		0.1681(14)
$\nu_6 + \nu_9$ (Δ)	4097.7537(50)	0.358(44)		0.0900(4)
$2\nu_8$ (Δ)	4094.4786(103)	0.351(85)		
$\nu_6 + \nu_7$ (Δ)	4092.9074(176)	1.419(145)		
$\nu_7 + \nu_8$ (Δ)	4095.8925(354)	0.355(290)		
$2\nu_6 + \nu_9$ (ϕ)	4098.9505(339)	0.372(303)		
Ground ^b	4084.74			0.0133

^aThe 2.5 σ uncertainties are given in parentheses for the last digits shown.

^bExtrapolated from the ν_6 and $2\nu_6$ state values.

Table 16.3. Molecular constants of 1,3-butadiyne (diacetylene-d₂) in excited vibrational states. [84037]

Parameter	Upper State ^a	Lower State ^a
$\nu_6 - \nu_8$ band	ν_6	ν_8
B_V (MHz)	3814.2822(15)	3812.9142(16)
D_V (kHz)	0.3113(128)	0.3149(113)
q_V (MHz)	2.2874(17)	2.2767(15)
ΔG_V (MHz)	86417.951(13)	
μ (D)	0.0450(11)	
	$\nu_6 + \nu_9$ (u)	$\nu_8 + \nu_9$ (g)
B_V (MHz) Σ^+	3824.3631(43)	3823.0200(44)
Σ^-	3824.4347(40)	3823.0598(43)
Δ	3824.3726(33)	3823.0410(36)
D_V (kHz) Σ^+	0.3439(731)	0.3469(674)
Σ^-	0.3493(388)	0.3519(381)
Δ	0.3182(283)	0.3197(278)
δG (MHz) $\Delta - \Sigma^+$	27847.(681)	53389.(681)
$\Delta - \Sigma^-$	32184.(2242)	30382.(2242)
ΔG (MHz) Σ^+	111358.561(38)	
Σ^-	84014.468(35)	
Δ	85816.240(33)	
q_9 (MHz)	4.898(240)	
q_6 (MHz)	2.2874 fixed	
q_8 (MHz)	2.2767 fixed	

^aValues in parentheses denote 2.5 standard deviations.

TABLE 16.4. Microwave spectrum of 1,3-butadiyne

C₄H₂

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' - J''$	Vib. state	Ref.
HCCCCH	10366.206	(0.050)	6 - 7	$1\nu_8 - 1\nu_6$	<i>f</i> [81046]
	10404.158	(0.050)	6 - 7	$1\nu_8 - 1\nu_6$	<i>e</i> [81046]
	15939.238	(0.050)	10 - 9	$1\nu_6 - 1\nu_8$	<i>e</i> [81036]
	15995.727	(0.050)	10 - 9	$1\nu_6 - 1\nu_8$	<i>f</i> [81046]
	19153.113	(0.050)	5 - 6	$1\nu_8 - 1\nu_6$	<i>f</i> [81046]
	19185.188	(0.050)	5 - 6	$1\nu_8 - 1\nu_6$	<i>e</i> [81046]
	19326.369	(0.050)	12 - 11	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>f</i> [82036]
	19343.214	(0.050)	12 - 11	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>e</i> [82036]
	23483.668	(0.050)	11 - 10	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^- [82036]
	24396.116	(0.050)	9 - 8	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [82036]
	24720.622	(0.050)	11 - 10	$1\nu_6 - 1\nu_8$	<i>e</i> [81046]
	24722.001	(0.050)	5 - 6	$1\nu_{8+9} - 1\nu_{6+9}$	Δ <i>e</i> [82036]
	24723.720	(0.050)	5 - 6	$1\nu_{8+9} - 1\nu_{6+9}$	Δ <i>f</i> [82036]
	24783.608	(0.050)	11 - 10	$1\nu_6 - 1\nu_8$	<i>f</i> [81046]
	27939.711	(0.050)	4 - 5	$1\nu_8 - 1\nu_6$	<i>f</i> [81046]
	27966.101	(0.050)	4 - 5	$1\nu_8 - 1\nu_6$	<i>e</i> [81046]
	28137.188	(0.050)	13 - 12	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>f</i> [82036]
	28160.648	(0.050)	13 - 12	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>e</i> [82036]
	28495.001	(0.050)	2 - 3	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [82036]
	29371.105	(0.050)	4 - 5	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [82036]
	32293.064	(0.050)	13 - 12	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^- [82036]
	33215.564	(0.050)	10 - 9	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [82036]
	33502.016	(0.050)	12 - 11	$1\nu_6 - 1\nu_8$	<i>e</i> [81046]
	33531.917	(0.050)	4 - 5	$1\nu_{8+9} - 1\nu_{6+9}$	Δ <i>e</i> [82036]
	33532.717	(0.050)	4 - 5	$1\nu_{8+9} - 1\nu_{6+9}$	Δ <i>f</i> [82036]
	33571.597	(0.050)	12 - 11	$1\nu_6 - 1\nu_8$	<i>f</i> [81046]
	36726.056	(0.050)	3 - 4	$1\nu_8 - 1\nu_6$	<i>f</i> [81046]
	36746.882	(0.050)	3 - 4	$1\nu_8 - 1\nu_6$	<i>e</i> [81046]
	36948.320	(0.050)	14 - 13	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>f</i> [82036]
	36980.115	(0.050)	14 - 13	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>e</i> [82036]
	38179.817	(0.050)	4 - 3	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [82036]
	41102.447	(0.050)	14 - 13	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^- [82036]
	42035.688	(0.050)	10 - 9	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [82036]
	42283.382	(0.050)	13 - 12	$1\nu_6 - 1\nu_8$	<i>e</i> [81046]
	42341.222	(0.050)	4 - 5	$1\nu_{8+9} - 1\nu_{6+9}$	Δ <i>e</i> [82036]
	42359.748	(0.050)	13 - 12	$1\nu_6 - 1\nu_8$	<i>f</i> [81046]
	45512.063	(0.050)	2 - 3	$1\nu_8 - 1\nu_6$	<i>f</i> [81046]
	45527.446	(0.050)	2 - 3	$1\nu_8 - 1\nu_6$	<i>e</i> [81046]
	46988.213	(0.050)	2 - 3	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [82036]
	49911.775	(0.050)	15 - 14	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^- [82036]
	50856.220	(0.050)	12 - 11	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [82036]
	51064.793	(0.050)	14 - 13	$1\nu_6 - 1\nu_8$	<i>e</i> [81046]
	51148.101	(0.050)	14 - 13	$1\nu_6 - 1\nu_8$	<i>f</i> [81046]
	51150.114	(0.050)	4 - 3	$1\nu_{8+9} - 1\nu_{6+9}$	Δ <i>f</i> [82036]
	54297.885	(0.050)	1 - 2	$1\nu_8 - 1\nu_6$	<i>f</i> [81046]
	54307.948	(0.050)	1 - 2	$1\nu_8 - 1\nu_6$	<i>e</i> [81046]
	54571.471	(0.050)	16 - 15	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>f</i> [82036]
	54626.336	(0.050)	16 - 15	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>e</i> [82036]
	54918.086	(0.050)	1 - 0	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [82036]
	55796.541	(0.050)	1 - 2	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [82036]
	58721.023	(0.050)	16 - 15	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^- [82036]
	59676.925	(0.050)	13 - 12	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [82036]
	59846.248	(0.050)	15 - 14	$1\nu_6 - 1\nu_8$	<i>e</i> [81046]
	59936.594	(0.050)	15 - 14	$1\nu_6 - 1\nu_8$	<i>f</i> [81046]
	63383.530	(0.050)	17 - 16	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>f</i> [82036]
	63453.736	(0.050)	17 - 16	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>e</i> [82036]
	63721.981	(0.050)	2 - 1	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [82036]
	64604.556	(0.050)	1 - 1	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [82036]
	67530.224	(0.050)	17 - 16	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^- [82036]
	68497.670	(0.050)	14 - 13	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [82036]
	68627.629	(0.050)	16 - 15	$1\nu_6 - 1\nu_8$	<i>e</i> [81046]
	68725.304	(0.050)	16 - 15	$1\nu_6 - 1\nu_8$	<i>f</i> [81046]
	71816.892	(0.050)	4 - 4	$1\nu_8 - 1\nu_6$	<i>ef</i> [81046]
	71837.647	(0.050)	3 - 3	$1\nu_8 - 1\nu_6$	<i>ef</i> [81046]
	71852.994	(0.050)	2 - 2	$1\nu_8 - 1\nu_6$	<i>e</i> [81046]
	71863.314	(0.050)	1 - 1	$1\nu_8 - 1\nu_6$	<i>ef</i> [81046]
	71873.102	(0.050)	1 - 1	$1\nu_8 - 1\nu_6$	<i>fe</i> [81046]

TABLE 16.4. Microwave spectrum of 1,3-butadiyne — Continued

C₄H₂

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' - J''$	Vib. state	Ref.
	71882.396	(0.050)	2 - 2	$1\nu_8 - 1\nu_6$	<i>fe</i> [81046]
	71896.242	(0.050)	3 - 3	$1\nu_8 - 1\nu_6$	<i>fe</i> [81046]
	71914.713	(0.050)	4 - 4	$1\nu_8 - 1\nu_6$	<i>fe</i> [81046]
	72195.871	(0.050)	18 - 17	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>f</i> [82036]
	72284.350	(0.050)	18 - 17	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>e</i> [82036]
	72524.001	(0.050)	3 - 2	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [82036]
	76339.339	(0.050)	18 - 17	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^- [82036]
	77317.949	(0.050)	15 - 14	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [82036]
	77409.181	(0.050)	17 - 16	$1\nu_6 - 1\nu_8$	<i>e</i> [82036]
	77514.202	(0.050)	17 - 16	$1\nu_6 - 1\nu_8$	<i>f</i> [82036]
	77570.815	(0.050)	4 - 4	$1\nu_{8+9} - 1\nu_{6+9}$	<i>fe</i> [82036]
	77572.418	(0.050)	3 - 3	$1\nu_{8+9} - 1\nu_{6+9}$	<i>ef</i> [82036]
	77573.323	(0.050)	2 - 2	$1\nu_{8+9} - 1\nu_{6+9}$	<i>fe</i> [82036]
	81008.656	(0.050)	19 - 18	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>f</i> [82036]
	81118.771	(0.050)	19 - 18	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>e</i> [82036]
	81324.066	(0.050)	3 - 2	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [82036]
	82219.760	(0.050)	1 - 0	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [82036]
	85148.237	(0.050)	19 - 18	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^- [82036]
	86137.441	(0.050)	16 - 15	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [82036]
	86190.631	(0.050)	18 - 17	$1\nu_6 - 1\nu_8$	<i>e</i> [82036]
	86303.186	(0.050)	18 - 17	$1\nu_6 - 1\nu_8$	<i>f</i> [82036]
	89428.244	(0.050)	2 - 1	$1\nu_8 - 1\nu_6$	<i>e</i> [82036]
	89437.861	(0.050)	2 - 1	$1\nu_8 - 1\nu_6$	<i>f</i> [82036]
	89821.699	(0.050)	10 - 19	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>f</i> [82036]
	89956.981	(0.050)	10 - 19	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>e</i> [82036]
	90122.305	(0.050)	5 - 4	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [82036]
	91026.942	(0.050)	2 - 1	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [82036]
	93956.940	(0.050)	20 - 19	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^- [82036]
	94955.928	(0.050)	17 - 16	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [82036]
	94972.022	(0.050)	19 - 18	$1\nu_6 - 1\nu_8$	<i>e</i> [82036]
	95092.267	(0.050)	19 - 18	$1\nu_6 - 1\nu_8$	<i>f</i> [82036]
	98635.136	(0.050)	21 - 20	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>f</i> [82036]
	98799.479	(0.050)	21 - 20	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>e</i> [82036]
	102765.404	(0.050)	21 - 20	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^- [82036]
	103753.379	(0.050)	20 - 19	$1\nu_6 - 1\nu_8$	<i>e</i> [82036]
	103773.020	(0.050)	18 - 17	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [82036]
	103881.484	(0.050)	20 - 19	$1\nu_6 - 1\nu_8$	<i>f</i> [82036]
	103995.578	(0.050)	3 - 2	$1\nu_{8+9} - 1\nu_{6+9}$	<i>e</i> [82036]
	106987.262	(0.050)	4 - 3	$1\nu_8 - 1\nu_6$	<i>e</i> [82036]
	107005.664	(0.050)	4 - 3	$1\nu_8 - 1\nu_6$	<i>f</i> [82036]
	107448.891	(0.050)	22 - 21	$1\nu_{6+9} - 1\nu_{8+9}$	<i>f</i> [82036]
	107646.637	(0.050)	22 - 21	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>e</i> [82036]
	107713.512	(0.050)	7 - 6	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [82036]
	108640.399	(0.050)	4 - 3	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [82036]
	111573.608	(0.050)	22 - 21	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^- [82036]
	112534.685	(0.050)	21 - 20	$1\nu_6 - 1\nu_8$	<i>e</i> [82036]
	112588.369	(0.050)	19 - 18	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [82036]
	112670.794	(0.050)	21 - 20	$1\nu_6 - 1\nu_8$	<i>f</i> [82036]
	112802.051	(0.050)	4 - 3	$1\nu_{8+9} - 1\nu_{6+9}$	<i>f</i> [82036]
	115766.433	(0.050)	5 - 4	$1\nu_8 - 1\nu_6$	<i>e</i> [82036]
	115789.016	(0.050)	5 - 4	$1\nu_8 - 1\nu_6$	<i>f</i> [82036]
	116263.138	(0.050)	23 - 22	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>f</i> [82036]
	116498.772	(0.050)	23 - 22	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>e</i> [82036]
	116506.680	(0.050)	8 - 7	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [82036]
	117446.561	(0.050)	5 - 4	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [82036]
	120381.531	(0.050)	23 - 22	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^- [82036]
	121315.959	(0.050)	22 - 21	$1\nu_6 - 1\nu_8$	<i>e</i> [82036]
	121401.629	(0.050)	20 - 19	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [82036]
	121460.178	(0.050)	22 - 21	$1\nu_6 - 1\nu_8$	<i>f</i> [82036]
	121608.007	(0.050)	5 - 4	$1\nu_{8+9} - 1\nu_{6+9}$	Δ <i>e</i> [82036]
	124545.399	(0.050)	6 - 5	$1\nu_8 - 1\nu_6$	<i>e</i> [82036]
	124572.043	(0.050)	6 - 5	$1\nu_8 - 1\nu_6$	<i>f</i> [82036]
	125077.626	(0.050)	24 - 23	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>f</i> [82036]
	125298.468	(0.050)	9 - 8	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [82036]
	125356.186	(0.050)	24 - 23	$1\nu_{6+9} - 1\nu_{8+9}$	Δ <i>e</i> [82036]
	126252.506	(0.050)	6 - 5	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [82036]
	129189.080	(0.050)	24 - 23	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^- [82036]

TABLE 16.4. Microwave spectrum of 1,3-butadiyne — Continued

C₄H₂

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' - J''$	Vib. state	Ref.
	130097.135	(0.050)	23 - 22	$1\nu_6 - 1\nu_8$	[82036]
	130212.435	(0.050)	21 - 20	$1\nu_{6+9} - 1\nu_{8+9}$	[82036]
	130249.652	(0.050)	23 - 22	$1\nu_6 - 1\nu_8$	[82036]
	130414.035	(0.050)	6 - 5	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	133324.095	(0.050)	7 - 6	$1\nu_8 - 1\nu_6$	[82036]
	133354.629	(0.050)	7 - 6	$1\nu_8 - 1\nu_6$	[82036]
	133892.550	(0.050)	25 - 24	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	134088.978	(0.050)	10 - 9	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	134219.116	(0.050)	25 - 24	$1\nu_{6+9} - 1\nu_{8+9}$	[82036]
	135058.018	(0.050)	7 - 6	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	139218.165	(0.050)	7 - 6	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	139219.435	(0.050)	7 - 6	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	142102.507	(0.050)	8 - 7	$1\nu_8 - 1\nu_6$	[82036]
	142136.842	(0.050)	8 - 7	$1\nu_8 - 1\nu_6$	[82036]
	142707.939	(0.050)	26 - 25	$1\nu_{6+9} - 1\nu_{8+9}$	[82036]
	142878.315	(0.050)	11 - 10	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	143088.041	(0.050)	26 - 25	$1\nu_{6+9} - 1\nu_{8+9}$	[82036]
	143863.183	(0.050)	8 - 7	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	148022.182	(0.050)	8 - 7	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	148024.537	(0.050)	8 - 7	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	150880.704	(0.050)	9 - 8	$1\nu_8 - 1\nu_6$	[82036]
	150918.629	(0.050)	9 - 8	$1\nu_8 - 1\nu_6$	[82036]
	151666.863	(0.050)	12 - 11	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	152667.962	(0.050)	9 - 8	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	156825.143	(0.050)	9 - 8	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	156829.215	(0.050)	9 - 8	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	159658.615	(0.050)	10 - 9	$1\nu_8 - 1\nu_6$	[82036]
	160454.614	(0.050)	13 - 12	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	161472.445	(0.050)	10 - 9	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	165627.043	(0.050)	10 - 9	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	165633.481	(0.050)	10 - 9	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	168436.178	(0.050)	11 - 10	$1\nu_8 - 1\nu_6$	[82036]
	168480.873	(0.050)	11 - 10	$1\nu_8 - 1\nu_6$	[82036]
	174427.490	(0.050)	11 - 10	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
	174437.376	(0.050)	11 - 10	$1\nu_{8+9} - 1\nu_{6+9}$	[82036]
HCCCD	40851.35	(0.05)	5 - 4	$1\nu_6$	[81047]
	40872.61	(0.05)	5 - 4	$1\nu_6$	[81047]
	40876.84	(0.05)	5 - 4	$2\nu_6$	[81047]
	40977.41	(0.05)	5 - 4	$1\nu_6, 1\nu_9$	[81047]
	49021.48	(0.05)	6 - 5	$1\nu_6$	[81047]
	49047.01	(0.05)	6 - 5	$1\nu_6$	[81047]
	49052.06	(0.05)	6 - 5	$2\nu_6$	[81047]
	49113.84	(0.05)	6 - 5	$1\nu_6, 1\nu_7$	[81047]
	49133.48	(0.05)	6 - 5	$2\nu_8$	[81047]
	49150.51	(0.05)	6 - 5	$1\nu_7, 1\nu_8$	[81047]
	49172.77	(0.05)	6 - 5	$1\nu_6, 1\nu_9$	[81047]
	49187.24	(0.05)	6 - 5	$2\nu_6, 1\nu_9$	[81047]
	57191.54	(0.05)	7 - 6	$1\nu_6$	[81047]
	57221.41	(0.05)	7 - 6	$1\nu_6$	[81047]
	57227.30	(0.05)	7 - 6	$2\nu_6$	[81047]
	57298.85	(0.05)	7 - 6	$1\nu_6, 1\nu_7$	[81047]
	57322.23	(0.05)	7 - 6	$2\nu_8$	[81047]
	57341.96	(0.05)	7 - 6	$1\nu_7, 1\nu_8$	[81047]
	57368.08	(0.05)	7 - 6	$1\nu_6, 1\nu_9$	[81047]
	57384.88	(0.05)	7 - 6	$2\nu_6, 1\nu_9$	[81047]
	65361.59	(0.05)	8 - 7	$1\nu_6$	[81047]
	65395.71	(0.05)	8 - 7	$1\nu_6$	[81047]
	65402.49	(0.05)	8 - 7	$2\nu_6$	[81047]
	65483.82	(0.05)	8 - 7	$1\nu_6, 1\nu_7$	[81047]
	65511.02	(0.05)	8 - 7	$2\nu_8$	[81047]
	65563.36	(0.05)	8 - 7	$1\nu_6, 1\nu_9$	[81047]
	65582.42	(0.05)	8 - 7	$2\nu_6, 1\nu_9$	[81047]
	73531.52	(0.05)	9 - 8	$1\nu_6$	[81047]
	73569.92	(0.05)	9 - 8	$1\nu_6$	[81047]
	73577.56	(0.05)	9 - 8	$2\nu_6$	[81047]
	73668.40	(0.05)	9 - 8	$1\nu_6, 1\nu_7$	[81047]
	73699.63	(0.05)	9 - 8	$2\nu_8$	[81047]

TABLE 16.4. Microwave spectrum of 1,3-butadiyne — Continued

C₄H₂

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' - J''$	Vib. state	Ref.
DCCCCD	73725.10	(0.05)	9 - 8	$1\nu_7, 1\nu_8$	[81047]
	73758.59	(0.05)	9 - 8	$1\nu_6, 1\nu_9$	[81047]
	73780.22	(0.05)	9 - 8	$2\nu_6, 1\nu_9$	[81047]
	32344.532	(0.050)	6 - 7	$1\nu_{6+9} - 1\nu_{8+9}$	Δf [84037]
	33077.941	(0.050)	6 - 7	$1\nu_6 - 1\nu_8$	f [84037]
	33109.382	(0.050)	6 - 7	$1\nu_6 - 1\nu_8$	e [84037]
	33516.980	(0.050)	19 - 18	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [84037]
	35016.295	(0.050)	9 - 10	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [84037]
	35227.837	(0.050)	16 - 15	$1\nu_8 - 1\nu_6$	e [84037]
	35298.118	(0.050)	16 - 15	$1\nu_8 - 1\nu_6$	f [84037]
	36167.930	(0.050)	16 - 15	$1\nu_{8+9} - 1\nu_{6+9}$	Δe [84037]
	36204.173	(0.050)	16 - 15	$1\nu_{8+9} - 1\nu_{6+9}$	Δf [84037]
	37984.890	(0.050)	16 - 15	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [84037]
	38179.389	(0.050)	5 - 6	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^- [84037]
	39974.857	(0.050)	5 - 6	$1\nu_{6+9} - 1\nu_{8+9}$	Δe [84037]
	40689.422	(0.050)	5 - 6	$1\nu_6 - 1\nu_8$	f [84037]
	40716.456	(0.050)	5 - 6	$1\nu_6 - 1\nu_8$	e [84037]
	41127.064	(0.050)	10 - 19	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [84037]
	42639.419	(0.050)	8 - 9	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [84037]
	42806.715	(0.050)	17 - 16	$1\nu_8 - 1\nu_6$	e [84037]
	42881.229	(0.050)	17 - 16	$1\nu_8 - 1\nu_6$	f [84037]
	43760.288	(0.050)	17 - 16	$1\nu_{8+9} - 1\nu_{6+9}$	Δe [84037]
	43807.142	(0.050)	17 - 16	$1\nu_{8+9} - 1\nu_{6+9}$	Δf [84037]
	45811.595	(0.050)	4 - 5	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^- [84037]
	45585.334	(0.050)	17 - 16	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [84037]
	47607.257	(0.050)	4 - 5	$1\nu_{6+9} - 1\nu_{8+9}$	Δf [84037]
	48303.674	(0.050)	4 - 5	$1\nu_6 - 1\nu_8$	f [84037]
	48326.218	(0.050)	4 - 5	$1\nu_6 - 1\nu_8$	e [84037]
	48737.095	(0.050)	21 - 20	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [84037]
	50264.776	(0.050)	7 - 8	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [84037]
	50382.694	(0.050)	18 - 17	$1\nu_8 - 1\nu_6$	e [84037]
	50461.391	(0.050)	18 - 17	$1\nu_8 - 1\nu_6$	f [84037]
	51347.882	(0.050)	18 - 17	$1\nu_{8+9} - 1\nu_{6+9}$	Δe [84037]
	51407.438	(0.050)	18 - 17	$1\nu_{8+9} - 1\nu_{6+9}$	Δf [84037]
	53182.728	(0.050)	18 - 17	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [84037]
	53446.647	(0.050)	18 - 17	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [84037]
	55242.595	(0.050)	3 - 4	$1\nu_{6+9} - 1\nu_{8+9}$	Δe [84037]
	55920.701	(0.050)	3 - 4	$1\nu_6 - 1\nu_8$	f [84037]
	55938.802	(0.050)	3 - 4	$1\nu_6 - 1\nu_8$	e [84037]
	56347.221	(0.050)	22 - 21	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [84037]
	57892.468	(0.050)	6 - 7	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [84037]
	57955.823	(0.050)	19 - 18	$1\nu_8 - 1\nu_6$	e [84037]
	58038.667	(0.050)	19 - 18	$1\nu_8 - 1\nu_6$	f [84037]
	58930.412	(0.050)	19 - 18	$1\nu_{8+9} - 1\nu_{6+9}$	Δe [84037]
	59004.969	(0.050)	19 - 18	$1\nu_{8+9} - 1\nu_{6+9}$	Δf [84037]
	60777.046	(0.050)	19 - 18	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [84037]
	61084.375	(0.050)	2 - 3	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^- [84037]
	62880.639	(0.050)	2 - 3	$1\nu_{6+9} - 1\nu_{8+9}$	Δf [84037]
	63540.539	(0.050)	2 - 3	$1\nu_6 - 1\nu_8$	f [84037]
	63554.142	(0.050)	2 - 3	$1\nu_6 - 1\nu_8$	e [84037]
63957.678	(0.050)	23 - 22	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [84037]	
65522.258	(0.050)	5 - 6	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [84037]	
65526.057	(0.050)	20 - 19	$1\nu_8 - 1\nu_6$	e [84037]	
65613.063	(0.050)	20 - 19	$1\nu_8 - 1\nu_6$	f [84037]	
66507.655	(0.050)	20 - 19	$1\nu_{8+9} - 1\nu_{6+9}$	Δe [84037]	
66599.864	(0.050)	20 - 19	$1\nu_{8+9} - 1\nu_{6+9}$	Δf [84037]	
68368.383	(0.050)	20 - 19	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [84037]	
68725.135	(0.050)	1 - 2	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^- [84037]	
71163.138	(0.050)	1 - 2	$1\nu_6 - 1\nu_8$	f [84037]	
71172.216	(0.050)	1 - 2	$1\nu_6 - 1\nu_8$	e [84037]	
71568.712	(0.050)	24 - 23	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [84037]	
73093.418	(0.050)	21 - 20	$1\nu_8 - 1\nu_6$	e [84037]	
73155.331	(0.050)	4 - 5	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [84037]	
73184.521	(0.050)	21 - 20	$1\nu_8 - 1\nu_6$	f [84037]	
74079.297	(0.050)	21 - 20	$1\nu_{8+9} - 1\nu_{6+9}$	Δe [84037]	
74191.989	(0.050)	21 - 20	$1\nu_{8+9} - 1\nu_{6+9}$	Δf [84037]	
75956.650	(0.050)	21 - 20	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [84037]	

TABLE 16.4. Microwave spectrum of 1,3-butadiyne — Continued

C₄H₂

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' - J''$	Vib. state	Ref.
	79180.490	(0.050)	25 - 24	$1\nu_{8+9} - 1\nu_{6+9}$ Σ^+	[84037]
	80657.824	(0.050)	22 - 21	$1\nu_8 - 1\nu_6$ e	[84037]
	80753.049	(0.050)	22 - 21	$1\nu_8 - 1\nu_6$ f	[84037]
	80790.589	(0.050)	3 - 4	$1\nu_{6+9} - 1\nu_{8+9}$ Σ^+	[84037]
	81645.035	(0.050)	22 - 21	$1\nu_{8+9} - 1\nu_{6+9}$ Δe	[84037]
	81781.383	(0.050)	22 - 21	$1\nu_{8+9} - 1\nu_{6+9}$ Δf	[84037]
	83541.884	(0.050)	22 - 21	$1\nu_{8+9} - 1\nu_{6+9}$ Σ^-	[84037]
	85818.945	(0.050)	2 - 2	$1\nu_{6+9} - 1\nu_{8+9}$ fe	[84037]
	85826.894	(0.050)	3 - 3	$1\nu_{6+9} - 1\nu_{8+9}$ ef	[84037]
	86411.081	(0.050)	2 - 2	$1\nu_6 - 1\nu_8$ ef	[84037]
	86414.742	(0.050)	1 - 1	$1\nu_6 - 1\nu_8$ ef	[84037]
	86423.868	(0.050)	1 - 1	$1\nu_6 - 1\nu_8$ fe	[84037]
	86438.408	(0.050)	2 - 2	$1\nu_6 - 1\nu_8$ fe	[84037]
	88428.528	(0.050)	2 - 3	$1\nu_{6+9} - 1\nu_{8+9}$ Σ^+	[84037]
	91663.350	(0.050)	1 - 0	$1\nu_{6+9} - 1\nu_{8+9}$ Σ^-	[84037]
	96069.222	(0.050)	1 - 2	$1\nu_{6+9} - 1\nu_{8+9}$ Σ^+	[84037]
	99314.932	(0.050)	2 - 1	$1\nu_{6+9} - 1\nu_{8+9}$ Σ^-	[84037]
	101671.864	(0.050)	2 - 1	$1\nu_6 - 1\nu_8$ e	[84037]
	101681.069	(0.050)	2 - 1	$1\nu_6 - 1\nu_8$ f	[84037]
	103712.513	(0.050)	0 - 1	$1\nu_{6+9} - 1\nu_{8+9}$ Σ^+	[84037]
	106969.288	(0.050)	3 - 2	$1\nu_{6+9} - 1\nu_{8+9}$ Σ^-	[84037]
	108765.215	(0.050)	3 - 2	$1\nu_{6+9} - 1\nu_{8+9}$ Δe	[84037]
	109303.585	(0.050)	3 - 2	$1\nu_6 - 1\nu_8$ e	[84037]
	109317.300	(0.050)	3 - 2	$1\nu_6 - 1\nu_8$ f	[84037]
	114626.348	(0.050)	4 - 3	$1\nu_{6+9} - 1\nu_{8+9}$ Σ^-	[84037]
	116421.888	(0.050)	4 - 3	$1\nu_{6+9} - 1\nu_{8+9}$ Δf	[84037]
	116938.002	(0.050)	4 - 3	$1\nu_6 - 1\nu_8$ e	[84037]
	116956.002	(0.050)	4 - 3	$1\nu_6 - 1\nu_8$ f	[84037]
	119007.306	(0.050)	1 - 0	$1\nu_{6+9} - 1\nu_{8+9}$ Σ^+	[84037]
	122286.102	(0.050)	5 - 4	$1\nu_{6+9} - 1\nu_{8+9}$ Σ^-	[84037]
	124081.088	(0.050)	5 - 4	$1\nu_{6+9} - 1\nu_{8+9}$ Δf	[84037]
	124081.895	(0.050)	5 - 4	$1\nu_{6+9} - 1\nu_{8+9}$ Δe	[84037]
	124575.054	(0.050)	5 - 4	$1\nu_6 - 1\nu_8$ e	[84037]
	124598.152	(0.050)	5 - 4	$1\nu_6 - 1\nu_8$ f	[84037]
	126658.622	(0.050)	2 - 1	$1\nu_{6+9} - 1\nu_{8+9}$ Σ^+	[84037]
	129948.152	(0.050)	6 - 5	$1\nu_{6+9} - 1\nu_{8+9}$ Σ^-	[84037]
	131743.177	(0.050)	6 - 5	$1\nu_{6+9} - 1\nu_{8+9}$ Δf	[84037]
	131744.522	(0.050)	6 - 5	$1\nu_{6+9} - 1\nu_{8+9}$ Δe	[84037]
	132214.860	(0.050)	6 - 5	$1\nu_6 - 1\nu_8$ e	[84037]
	132242.665	(0.050)	6 - 5	$1\nu_6 - 1\nu_8$ f	[84037]
	134312.637	(0.050)	3 - 2	$1\nu_{6+9} - 1\nu_{8+9}$ Σ^+	[84037]
	137613.722	(0.050)	7 - 6	$1\nu_{6+9} - 1\nu_{8+9}$ Σ^-	[84037]
	139407.832	(0.050)	7 - 6	$1\nu_{6+9} - 1\nu_{8+9}$ Δf	[84037]
	139410.194	(0.050)	7 - 6	$1\nu_{6+9} - 1\nu_{8+9}$ Δe	[84037]
	139857.357	(0.050)	7 - 6	$1\nu_6 - 1\nu_8$ e	[84037]
	139889.795	(0.050)	7 - 6	$1\nu_6 - 1\nu_8$ f	[84037]
	141969.201	(0.050)	4 - 3	$1\nu_{6+9} - 1\nu_{8+9}$ Σ^+	[84037]
	145281.547	(0.050)	8 - 7	$1\nu_{6+9} - 1\nu_{8+9}$ Σ^-	[84037]
	147074.973	(0.050)	8 - 7	$1\nu_{6+9} - 1\nu_{8+9}$ Δf	[84037]
	147079.000	(0.050)	8 - 7	$1\nu_{6+9} - 1\nu_{8+9}$ Δe	[84037]
	147502.487	(0.050)	8 - 7	$1\nu_6 - 1\nu_8$ e	[84037]
	147539.698	(0.050)	8 - 7	$1\nu_6 - 1\nu_8$ f	[84037]
	149628.128	(0.050)	5 - 4	$1\nu_{6+9} - 1\nu_{8+9}$ Σ^+	[84037]

Table 17.1. Rotational constants for the ground, the $\nu_{13}=1$ and the $\nu_{18}=1$ states of 1-butene-3-yne and 1-butene-3-yne-4d.

Parameter	Ground State	$\nu_{13} = 1$	$\nu_{18} = 1$	Ground State	$\nu_{13} = 1$	$\nu_{18} = 1$
<u>Rotational Constants [80032]</u>						
A (MHz)	50308.(55)	49274.(59)	51676.(53)	49393.(34)	48337.(36)	50866.(49)
B (MHz)	4744.9317(77)	4763.276(11)	4747.7146(81)	4403.9538(40)	4420.6331(43)	4406.1168(51)
C (MHz)	4329.7899(77)	4337.5385(99)	4338.6433(83)	4037.8007(40)	4044.8607(43)	4045.6294(51)
D_J (kHz)	1.93(22)	2.17(28)	1.86(21)	1.56(11)	1.60(12)	1.60(14)
D_{JK} (kHz)	-83.22(67)	-70.90(86)	-93.19(64)	-77.35(34)	-66.43(46)	-88.66(44)
<u>Electric Dipole Moment [70061]</u>						
μ_a (D)	0.223(20)			0.206(8)		
μ_b (D)	0.02			0.02		

Table 17.2. Rotational analysis for the ground state of 1-butene-3-yne in the present work.

Parameter	$\text{CH}_2=\text{CHC}\equiv\text{CH}$
A'' (MHz)	50291.4(107)
B'' (MHz)	4744.872(5)
C'' (MHz)	4329.687(5)
τ_1 (MHz)	0.31029(46)
τ_2 (MHz)	0.01873(37)
τ_3^a (MHz)	1.119(88)
τ_{bbbb} (MHz)	-0.01055(39)
τ_{cccc} (MHz)	-0.00449(36)

^aThe value of τ_3 is derived from the planarity conditions.

TABLE 17.3. Microwave spectrum of 1-butene-3-yne

C₄H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
CH ₂ CHCCH	9074.740	(0.020)	1(0, 1) - 0(0, 0)		[70061]
	9086.30	(0.02)	1(0, 1) - 0(0, 0)	1ν ₁₈	[70061]
	9100.73	(0.02)	1(0, 1) - 0(0, 0)	1ν ₁₃	[70061]
	9113.0	(0.1)	1(0, 1) - 0(0, 0)	1ν ₁₃ , 1ν ₁₈	[70061]
	9127.5	(0.1)	1(0, 1) - 0(0, 0)	2ν ₁₃	[70061]
	17734.530	(0.020)	2(1, 2) - 1(1, 1)		[70061]
	17763.05	(0.02)	2(1, 2) - 1(1, 1)	1ν ₁₈	[70061]
	17776.05	(0.02)	2(1, 2) - 1(1, 1)	1ν ₁₃	[70061]
	17794.0	(0.3)	2(1, 2) - 1(1, 1)	2ν ₁₈	[70061]
	17806.5	(0.1)	2(1, 2) - 1(1, 1)	1ν ₁₃ , 1ν ₁₈	[70061]
	17816.5	(0.1)	2(1, 2) - 1(1, 1)	2ν ₁₃	[70061]
	18146.580	(0.020)	2(0, 2) - 1(0, 1)		[70061]
	18169.97	(0.02)	2(0, 2) - 1(0, 1)	1ν ₁₈	[70061]
	18198.58	(0.02)	2(0, 2) - 1(0, 1)	1ν ₁₃	[70061]
	18221.1	(0.1)	2(0, 2) - 1(0, 1)	1ν ₁₃ , 1ν ₁₈	[70061]
	18429.1	(0.1)	2(0, 2) - 1(0, 1)	2ν ₁₃	[70061]
	18564.910	(0.020)	2(1, 1) - 1(1, 0)		[70061]
	18582.16	(0.02)	2(1, 1) - 1(1, 0)	1ν ₁₈	[70061]
	18600.3	(0.3)	2(1, 1) - 1(1, 0)	2ν ₁₈	[70061]
	18627.64	(0.02)	2(1, 1) - 1(1, 0)	1ν ₁₃	[70061]
	18643.0	(0.2)	2(1, 1) - 1(1, 0)	1ν ₁₃ , 1ν ₁₈	[70061]
	18689.3	(0.1)	2(1, 1) - 1(1, 0)	2ν ₁₃	[70061]
	26599.930	(0.020)	3(1, 3) - 2(1, 2)		[70061]
	26644.19	(0.02)	3(1, 3) - 2(1, 2)	1ν ₁₈	[70061]
	26662.18	(0.02)	3(1, 3) - 2(1, 2)	1ν ₁₃	[70061]
	26688.0	(0.3)	3(1, 3) - 2(1, 2)	2ν ₁₈	[70061]
	26707.0	(0.1)	3(1, 3) - 2(1, 2)	1ν ₁₃ , 1ν ₁₈	[70061]
	26723.00	(0.05)	3(1, 3) - 2(1, 2)	2ν ₁₃	[70061]
	27212.620	(0.020)	3(0, 3) - 2(0, 2)		[70061]
	27225.990	(0.020)	3(2, 2) - 2(2, 1)		[70061]
	27237.270	(0.020)	3(2, 1) - 2(2, 0)		[70061]
	27248.22	(0.02)	3(0, 3) - 2(0, 2)	1ν ₁₈	[70061]
	27261.07	(0.02)	3(2, 2) - 2(2, 1)	1ν ₁₈	[70061]
	27271.76	(0.03)	3(2, 1) - 2(2, 0)	1ν ₁₈	[70061]
	27290.06	(0.02)	3(0, 3) - 2(0, 2)	1ν ₁₃	[70061]
	27303.86	(0.02)	3(2, 2) - 2(2, 1)	1ν ₁₃	[70061]
	27316.07	(0.02)	3(2, 1) - 2(2, 0)	1ν ₁₃	[70061]
	27365.77	(0.05)	3(0, 3) - 2(0, 2)	2ν ₁₃	[70061]
	27380.29	(0.05)	3(2, 2) - 2(2, 1)	2ν ₁₃	[70061]
	27392.95	(0.05)	3(2, 1) - 2(2, 0)	2ν ₁₃	[70061]
	27845.380	(0.020)	3(1, 2) - 2(1, 1)		[70061]
	27871.38	(0.02)	3(1, 2) - 2(1, 1)	1ν ₁₈	[70061]
	27898.0	(0.3)	3(1, 2) - 2(1, 1)	2ν ₁₈	[70061]
	27939.32	(0.02)	3(1, 2) - 2(1, 1)	1ν ₁₃	[70061]
	27961.70	(0.05)	3(1, 2) - 2(1, 1)	1ν ₁₃ , 1ν ₁₈	[70061]
	28031.60	(0.05)	3(1, 2) - 2(1, 1)	2ν ₁₃	[70061]
	35463.220	(0.050)	4(1, 4) - 3(1, 3)		[80032]
	35522.305	(0.050)	4(1, 4) - 3(1, 3)	1ν ₁₈	[80032]
	35545.760	(0.050)	4(1, 4) - 3(1, 3)	1ν ₁₃	[80032]
	36270.165	(0.050)	4(0, 4) - 3(0, 3)		[80032]
	36298.870	(0.050)	4(2, 3) - 3(2, 2)		[80032]
	36310.025	(0.10)	4(3, 1) - 3(3, 0)		[80032]
	36310.025	(0.10)	4(3, 2) - 3(3, 1)		[80032]
	36318.335	(0.050)	4(0, 4) - 3(0, 3)	1ν ₁₈	[80032]
	36327.075	(0.050)	4(2, 2) - 3(2, 1)		[80032]
	36345.890	(0.050)	4(2, 3) - 3(2, 2)	1ν ₁₈	[80032]
	36356.990	(0.050)	4(3, 1) - 3(3, 0)	1ν ₁₈	[80032]
	36356.990	(0.050)	4(3, 2) - 3(3, 1)	1ν ₁₈	[80032]
	36372.310	(0.050)	4(0, 4) - 3(0, 3)	1ν ₁₃	[80032]
	36372.480	(0.050)	4(2, 2) - 3(2, 1)	1ν ₁₈	[80032]
	36402.620	(0.050)	4(2, 3) - 3(2, 2)	1ν ₁₃	[80032]
	36413.893	(0.050)	4(3, 1) - 3(3, 0)	1ν ₁₃	[80032]
	36413.893	(0.050)	4(3, 2) - 3(3, 1)	1ν ₁₃	[80032]
	36432.990	(0.050)	4(2, 2) - 3(2, 1)	1ν ₁₃	[80032]
	37123.640	(0.050)	4(1, 3) - 3(1, 2)		[80032]
	37158.465	(0.050)	4(1, 3) - 3(1, 2)	1ν ₁₈	[80032]
	37248.615	(0.050)	4(1, 3) - 3(1, 2)	1ν ₁₃	[80032]

TABLE 17.3. Microwave spectrum of 1-butene-3-yne — Continued

C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	63362.840	(0.050)	7(0, 7) - 6(0, 6)		[77036]
	63503.250	(0.050)	7(2, 6) - 6(2, 5)		[77036]
	63555.250	(0.100)	7(3, 4) - 6(3, 3)		[77036]
	63559.630	(0.100)	7(5, 2) - 6(5, 1)		[77036]
	63660.820	(0.050)	7(2, 5) - 6(2, 4)		[77036]
	64936.590	(0.100)	7(1, 6) - 6(1, 5)		[77036]
	88558.980	(0.130)	10(1, 10) - 9(1, 9)		[77036]
	90279.350	(0.130)	10(0, 10) - 9(0, 9)		[77036]
	90675.270	(0.070)	10(2, 9) - 9(2, 8)		[77036]
	90802.530	(0.070)	10(4, 7) - 9(4, 6)		[77036]
	90805.710	(0.070)	10(5, 5) - 9(5, 4)		[77036]
	90813.630	(0.070)	10(3, 8) - 9(3, 7)		[77036]
	90817.790	(0.050)	10(6, 4) - 9(6, 3)		[77036]
	90823.130	(0.070)	10(3, 7) - 9(3, 6)		[77036]
	90835.610	(0.070)	10(7, 3) - 9(7, 2)		[77036]
	90858.100	(0.070)	10(8, 2) - 9(8, 1)		[77036]
	90884.550	(0.070)	10(9, 1) - 9(9, 0)		[77036]
	91135.390	(0.070)	10(2, 8) - 9(2, 7)		[77036]
CH ₂ CHCCD	8441.741	(0.050)	1(0, 1) - 0(0, 0)		[80032]
	8451.730	(0.050)	1(0, 1) - 0(0, 0)	1ν ₁₈	[80032]
	8465.504	(0.050)	1(0, 1) - 0(0, 0)	1ν ₁₃	[80032]
	8489.0	(0.1)	1(0, 1) - 0(0, 0)	2ν ₁₃	[70061]
	8512.0	(0.1)	1(0, 1) - 0(0, 0)	3ν ₁₃	[70061]
	16517.602	(0.050)	2(1, 2) - 1(1, 1)		[80032]
	16543.265	(0.050)	2(1, 2) - 1(1, 1)	1ν ₁₈	[80032]
	16555.400	(0.050)	2(1, 2) - 1(1, 1)	1ν ₁₃	[80032]
	16569.0	(0.3)	2(1, 2) - 1(1, 1)	2ν ₁₈	[70061]
	16592.5	(0.2)	2(1, 2) - 1(1, 1)	2ν ₁₃	[70061]
	16881.231	(0.050)	2(0, 2) - 1(0, 1)		[80032]
	16901.368	(0.050)	2(0, 2) - 1(0, 1)	1ν ₁₈	[80032]
	16922.0	(0.3)	2(0, 2) - 1(0, 1)	2ν ₁₈	[70061]
	16928.523	(0.050)	2(0, 2) - 1(0, 1)	1ν ₁₃	[80032]
	16975.5	(0.2)	2(0, 2) - 1(0, 1)	2ν ₁₃	[70061]
	17019.5	(0.2)	2(0, 2) - 1(0, 1)	3ν ₁₃	[70061]
	17249.939	(0.050)	2(1, 1) - 1(1, 0)		[80032]
	17264.280	(0.050)	2(1, 1) - 1(1, 0)	1ν ₁₈	[80032]
	17279.5	(0.3)	2(1, 1) - 1(1, 0)	2ν ₁₈	[70061]
	17307.000	(0.050)	2(1, 1) - 1(1, 0)	1ν ₁₃	[80032]
	17362.3	(0.3)	2(1, 1) - 1(1, 0)	2ν ₁₃	[70061]
	17418.7	(0.3)	2(1, 1) - 1(1, 0)	3ν ₁₃	[70061]
	24774.933	(0.050)	3(1, 3) - 2(1, 2)		[80032]
	24813.560	(0.050)	3(1, 3) - 2(1, 2)	1ν ₁₈	[80032]
	24831.552	(0.050)	3(1, 3) - 2(1, 2)	1ν ₁₃	[80032]
	24853.1	(0.3)	3(1, 3) - 2(1, 2)	2ν ₁₈	[70061]
	24886.5	(0.3)	3(1, 3) - 2(1, 2)	2ν ₁₃	[70061]
	24942.1	(0.3)	3(1, 3) - 2(1, 2)	3ν ₁₃	[70061]
	25316.186	(0.050)	3(0, 3) - 2(0, 2)		[80032]
	25326.982	(0.050)	3(2, 2) - 2(2, 1)		[80032]
	25335.828	(0.050)	3(2, 1) - 2(2, 0)		[80032]
	25346.700	(0.050)	3(0, 3) - 2(0, 2)	1ν ₁₈	[80032]
	25357.249	(0.050)	3(2, 2) - 2(2, 1)	1ν ₁₈	[80032]
	25365.538	(0.050)	3(2, 1) - 2(2, 0)	1ν ₁₈	[80032]
	25386.704	(0.050)	3(0, 3) - 2(0, 2)	1ν ₁₃	[80032]
	25397.912	(0.050)	3(2, 2) - 2(2, 1)	1ν ₁₃	[80032]
	25407.487	(0.050)	3(2, 1) - 2(2, 0)	1ν ₁₃	[80032]
	25468.3	(0.5)	3(2, 2) - 2(2, 1)	2ν ₁₃	[70061]
	25476.5	(0.5)	3(2, 1) - 2(2, 0)	2ν ₁₃	[70061]
	25536.8	(0.5)	3(2, 2) - 2(2, 1)	3ν ₁₃	[70061]
	25546.0	(0.5)	3(2, 1) - 2(2, 0)	3ν ₁₃	[70061]
	25873.410	(0.050)	3(1, 2) - 2(1, 1)		[80032]
	25895.031	(0.050)	3(1, 2) - 2(1, 1)	1ν ₁₈	[80032]
	25918.3	(0.3)	3(1, 2) - 2(1, 1)	2ν ₁₈	[70061]
	25958.880	(0.050)	3(1, 2) - 2(1, 1)	1ν ₁₃	[80032]
	26043.3	(0.3)	3(1, 2) - 2(1, 1)	2ν ₁₃	[70061]
	26125.3	(0.5)	3(1, 2) - 2(1, 1)	3ν ₁₃	[70061]
	33030.523	(0.050)	4(1, 4) - 3(1, 3)		[80032]
	33082.178	(0.050)	4(1, 4) - 3(1, 3)	1ν ₁₈	[80032]

TABLE 17.3. Microwave spectrum of 1-butene-3-yne — Continued

C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	33105.801	(0.050)	4(1, 4) - 3(1, 3)	1 ν_{13}	[80032]
	33179.8	(0.3)	4(1, 4) - 3(1, 3)	2 ν_{13}	[70061]
	33251.7	(0.3)	4(1, 4) - 3(1, 3)	3 ν_{13}	[70061]
	33744.355	(0.050)	4(0, 4) - 3(0, 3)		[80032]
	33767.383	(0.050)	4(2, 3) - 3(2, 2)		[80032]
	33776.635	(0.050)	4(3, 2) - 3(3, 1)		[80032]
	33776.635	(0.050)	4(3, 1) - 3(3, 0)		[80032]
	33785.663	(0.050)	4(0, 4) - 3(0, 3)	1 ν_{18}	[80032]
	33789.618	(0.050)	4(2, 2) - 3(2, 1)		[80032]
	33807.800	(0.050)	4(2, 3) - 3(2, 2)	1 ν_{18}	[80032]
	33817.130	(0.050)	4(3, 2) - 3(3, 1)	1 ν_{18}	[80032]
	33817.130	(0.050)	4(3, 1) - 3(3, 0)	1 ν_{18}	[80032]
	33828.670	(0.050)	4(2, 2) - 3(2, 1)	1 ν_{18}	[80032]
	33837.553	(0.050)	4(0, 4) - 3(0, 3)	1 ν_{13}	[80032]
	33861.830	(0.050)	4(2, 3) - 3(2, 2)	1 ν_{13}	[80032]
	33871.151	(0.050)	4(3, 2) - 3(3, 1)	1 ν_{13}	[80032]
	33871.151	(0.050)	4(3, 1) - 3(3, 0)	1 ν_{13}	[80032]
	33885.830	(0.050)	4(2, 2) - 3(2, 1)	1 ν_{13}	[80032]
	33955.0	(0.5)	4(2, 3) - 3(2, 2)	2 ν_{13}	[70061]
	33964.0	(0.5)	4(3, 2) - 3(3, 1)	2 ν_{13}	[70061]
	33964.0	(0.5)	4(3, 1) - 3(3, 0)	2 ν_{13}	[70061]
	33980.3	(0.5)	4(2, 2) - 3(2, 1)	2 ν_{13}	[70061]
	34495.050	(0.050)	4(1, 3) - 3(1, 2)		[80032]
	34524.050	(0.050)	4(1, 3) - 3(1, 2)	1 ν_{18}	[80032]
	34554.0	(0.3)	4(1, 3) - 3(1, 2)	2 ν_{18}	[70061]
	34608.790	(0.050)	4(1, 3) - 3(1, 2)	1 ν_{13}	[80032]
	34720.0	(0.3)	4(1, 3) - 3(1, 2)	2 ν_{13}	[70061]
	34831.0	(0.3)	4(1, 3) - 3(1, 2)	3 ν_{13}	[70061]

Table 18.1. Molecular constants for methylene cyclopropene and its ¹³C isotopic forms. [86013]

Parameter	HC=CHC=CH ₂	H ¹³ C=CHC=CH ₂	HC=CHC= ¹³ CH ₂
<u>Rotational Constants</u>			
A (MHz)	29294.60(103)	28618.83(1019)	29322.21(1599)
B (MHz)	7154.36(6)	7055.65(2)	6903.74(5)
C (MHz)	5744.23(6)	5653.55(2)	5581.52(5)
Δ (u Å ²)	0.0894	0.1048	0.1059
<u>Electric Dipole Moment</u>			
μ _a (D)	1.90(2)		

TABLE 18.2. Microwave spectrum of methylenecyclopropene

C₄H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.	
$\begin{array}{c} \text{CHCHCCH}_2 \\ \square \\ \text{CH}_2 \\ \\ \text{C} \\ / \backslash \\ \text{HC}=\text{CH} \end{array}$	27207.47	(0.10)	2(1, 1) - 1(1, 0)	[86013]	
	29454.45	(0.10)	6(1, 5) - 6(1, 6)	[86013]	
	34760.46	(0.10)	11(2, 9) - 11(2, 10)	[86013]	
	35015.64	(0.10)	16(3, 13) - 16(3, 14)	[86013]	
	36540.88	(0.10)	3(1, 3) - 2(1, 2)	[86013]	
	38436.00	(0.10)	3(0, 3) - 2(0, 2)	[86013]	
	38695.53	(0.10)	3(2, 2) - 2(2, 1)	[86013]	
	38955.44	(0.10)	3(2, 1) - 2(2, 0)	[86013]	
	¹³ CHCHCCH ₂	26820.73	(0.10)	2(1, 1) - 1(1, 0)	[86013]
		29281.19	(0.10)	6(1, 5) - 6(1, 6)	[86013]
35984.12		(0.10)	3(1, 3) - 2(1, 2)	[86013]	
37863.85		(0.10)	3(0, 3) - 2(0, 2)	[86013]	
38127.43		(0.10)	3(2, 2) - 2(2, 1)	[86013]	
CHCHC ¹³ CH ₂	38391.30	(0.10)	3(2, 1) - 2(2, 0)	[86013]	
	35437.85	(0.10)	3(1, 3) - 2(1, 2)	[86013]	
	37229.35	(0.10)	3(0, 3) - 2(0, 2)	[86013]	
	37455.56	(0.10)	3(2, 2) - 2(2, 1)	[86013]	
	37682.22	(0.10)	3(2, 1) - 2(2, 0)	[86013]	
	39402.98	(0.10)	3(1, 2) - 2(1, 1)	[86013]	

Table 19.1. Molecular constants for 2-butyne-1,1,1-d₃ (dimethyl acetylene). [84027]

Parameter	Value ^a
B (MHz)	2982.4980(11)
D _J (kHz)	0.2570(9)
D _{JK} (kHz)	9.776(12)
G (kHz)	-93.90(11)
L (kHz)	25.97(6)
C (kHz)	-38.2(1)
s ² L (kHz)	2.65(15)
s ^b	0.319(9)
v ₃ ^b (cm ⁻¹)	5.62(16)
F ^b (kHz)	-123.2(75)

^aThe uncertainties are 2.5 times standard deviations. See reference [84027] for definition of parameters.
^bDerived from other constants.

TABLE 19.2. Microwave spectrum of 2-butyne-1,1,1-d₃C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'K'm'_H - J''K''m''_H$	Ref.
CH ₃ CCCD ₃	89446.00	(0.05)	15 0 3 - 14 0 3	[84027]
	89458.51	(0.05)	15 2 3 - 14 2 3	[84027]
	89458.51	(0.05)	15 4 0 - 14 4 0	[84027]
	89459.52	(0.05)	15 7 3 - 14 7 3	[84027]
	89459.52	(0.05)	15 2-1 - 14 2-1	[84027]
	89462.03	(0.05)	15 3 3 - 14 3 3	[84027]
	89463.94	(0.05)	15 1 2 - 14 1 2	[84027]
	89463.94	(0.05)	15 3 0 - 14 3 0	[84027]
	89464.63	(0.05)	15 5 3 - 14 5 3	[84027]
	89470.64	(0.05)	15 1 1 - 14 1 1	[84027]
	89470.64	(0.05)	15 1 0 - 14 1 0	[84027]
	89470.64	(0.05)	15 2 1 - 14 2 1	[84027]
	89471.60	(0.05)	15 0 0 - 14 0 0	[84027]
	113281.20	(0.05)	19 6 6 - 18 6 6	[84027]
	113283.10	(0.05)	19 1 4 - 18 1 4	[84027]
	113283.60	(0.05)	19 3-2 - 18 3-2	[84027]
	113284.50	(0.05)	19 1-3 - 18 1-3	[84027]
	113287.10	(0.05)	19 7 6 - 18 7 6	[84027]
	113288.10	(0.05)	19 6 0 - 18 6 0	[84027]
	113290.90	(0.05)	19 8 6 - 18 8 6	[84027]
	113292.30	(0.05)	19 9 6 - 18 9 6	[84027]
	113293.30	(0.05)	19 4-1 - 18 4-1	[84027]
	113293.30	(0.05)	19 2 4 - 18 2 4	[84027]
	113295.63	(0.05)	19 0 3 - 18 0 3	[84027]
	113300.15	(0.05)	19 6 5 - 18 6 5	[84027]
	113300.15	(0.05)	19 5 0 - 18 5 0	[84027]
	113301.07	(0.05)	19 3 4 - 18 3 4	[84027]
	113301.07	(0.05)	19 9 5 - 18 9 5	[84027]
	113304.04	(0.05)	19 3-1 - 18 3-1	[84027]
	113304.71	(0.05)	19 1 3 - 18 1 3	[84027]
	113305.60	(0.05)	19 1-2 - 18 1-2	[84027]
	113306.43	(0.05)	19 8 3 - 18 8 3	[84027]
	113307.03	(0.05)	19 7 2 - 18 7 2	[84027]
	113307.03	(0.05)	19 4 4 - 18 4 4	[84027]
	113308.30	(0.05)	19 8 4 - 18 8 4	[84027]
	113309.86	(0.05)	19 7 4 - 18 7 4	[84027]
	113310.63	(0.05)	19 5 4 - 18 5 4	[84027]
	113311.49	(0.05)	19 2 3 - 18 2 3	[84027]
	113311.49	(0.05)	19 4 0 - 18 4 0	[84027]
	113312.68	(0.05)	19 7 3 - 18 7 3	[84027]
	113312.68	(0.05)	19 2-1 - 18 2-1	[84027]
	113313.44	(0.05)	19 0 2 - 18 0 2	[84027]
	113313.96	(0.05)	19 5 1 - 18 5 1	[84027]
	113314.67	(0.05)	19 6 2 - 18 6 2	[84027]
	113315.95	(0.05)	19 3 3 - 18 3 3	[84027]
	113317.11	(0.05)	19 6 3 - 18 6 3	[84027]
	113317.60	(0.05)	19 4 3 - 18 4 3	[84027]
	113318.32	(0.05)	19 1 2 - 18 1 2	[84027]
	113318.32	(0.05)	19 3 0 - 18 3 0	[84027]
	113319.20	(0.05)	19 5 3 - 18 5 3	[84027]
	113319.90	(0.05)	19 5 2 - 18 5 2	[84027]
	113320.40	(0.05)	19 4 1 - 18 4 1	[84027]
	113320.80	(0.05)	19 1-1 - 18 1-1	[84027]
	113323.21	(0.05)	19 2 2 - 18 2 2	[84027]
	113323.21	(0.05)	19 4 2 - 18 4 2	[84027]
	113323.70	(0.05)	19 2 0 - 18 2 0	[84027]
	113324.13	(0.05)	19 3 2 - 18 3 2	[84027]
	113324.65	(0.05)	19 0 1 - 18 0 1	[84027]
	113324.65	(0.05)	19 3 1 - 18 3 1	[84027]
	113326.89	(0.05)	19 1 1 - 18 1 1	[84027]
	113326.89	(0.05)	19 1 0 - 18 1 0	[84027]
	113326.89	(0.05)	19 2 1 - 18 2 1	[84027]
	113328.04	(0.05)	19 0 0 - 18 0 0	[84027]
	137125.90	(0.05)	23 6 6 - 22 6 6	[84027]
	137128.30	(0.05)	23 1 4 - 22 1 4	[84027]
	137128.80	(0.05)	23 3-2 - 22 3-2	[84027]
	137129.90	(0.05)	23 1-3 - 22 1-3	[84027]

TABLE 19.2. Microwave spectrum of 2-butyne-1,1,1-d₃ — ContinuedC₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'K'm'_l - J''K''m''_l$	Ref.
	137133.10	(0.05)	23 7 6 - 22 7 6	[84027]
	137134.30	(0.05)	23 6 0 - 22 6 0	[84027]
	137137.60	(0.05)	23 8 6 - 22 8 6	[84027]
	137139.40	(0.05)	23 9 6 - 22 9 6	[84027]
	137140.40	(0.05)	23 4 -1 - 22 4 -1	[84027]
	137140.40	(0.05)	23 2 4 - 22 2 4	[84027]
	137143.39	(0.05)	23 0 3 - 22 0 3	[84027]
	137145.45	(0.05)	23 8 2 - 22 8 2	[84027]
	137146.10	(0.05)	23 9 3 - 22 9 3	[84027]
	137148.86	(0.05)	23 5 0 - 22 5 0	[84027]
	137148.86	(0.05)	23 6 5 - 22 6 5	[84027]
	137149.99	(0.05)	23 3 4 - 22 3 4	[84027]
	137149.99	(0.05)	23 9 5 - 22 9 5	[84027]
	137153.64	(0.05)	23 3 -1 - 22 3 -1	[84027]
	137154.37	(0.05)	23 1 3 - 22 1 3	[84027]
	137155.51	(0.05)	23 1 -2 - 22 1 -2	[84027]
	137156.45	(0.05)	23 8 3 - 22 8 3	[84027]
	137157.23	(0.05)	23 4 4 - 22 4 4	[84027]
	137157.23	(0.05)	23 7 2 - 22 7 2	[84027]
	137158.74	(0.05)	23 8 4 - 22 8 4	[84027]
	137160.60	(0.05)	23 7 4 - 22 7 4	[84027]
	137161.46	(0.05)	23 5 4 - 22 5 4	[84027]
	137162.54	(0.05)	23 2 3 - 22 2 3	[84027]
	137162.54	(0.05)	23 4 0 - 22 4 0	[84027]
	137164.08	(0.05)	23 2 -1 - 22 2 -1	[84027]
	137164.08	(0.05)	23 7 3 - 22 7 3	[84027]
	137164.84	(0.05)	23 0 2 - 22 0 2	[84027]
	137165.56	(0.05)	23 5 1 - 22 5 1	[84027]
	137166.21	(0.05)	23 6 2 - 22 6 2	[84027]
	137167.96	(0.05)	23 3 3 - 22 3 3	[84027]
	137169.29	(0.05)	23 6 3 - 22 6 3	[84027]
	137169.90	(0.05)	23 4 3 - 22 4 3	[84027]
	137170.85	(0.05)	23 1 2 - 22 1 2	[84027]
	137170.85	(0.05)	23 3 0 - 22 3 0	[84027]
	137171.82	(0.05)	23 5 3 - 22 5 3	[84027]
	137172.81	(0.05)	23 5 2 - 22 5 2	[84027]
	137173.32	(0.05)	23 4 1 - 22 4 1	[84027]
	137173.73	(0.05)	23 1 -1 - 22 1 -1	[84027]
	137176.74	(0.05)	23 2 2 - 22 2 2	[84027]
	137176.74	(0.05)	23 4 2 - 22 4 2	[84027]
	137177.33	(0.05)	23 2 0 - 22 2 0	[84027]
	137177.94	(0.05)	23 3 2 - 22 3 2	[84027]
	137178.50	(0.05)	23 0 1 - 22 0 1	[84027]
	137178.50	(0.05)	23 3 1 - 22 3 1	[84027]
	137181.18	(0.05)	23 1 1 - 22 1 1	[84027]
	137181.18	(0.05)	23 1 0 - 22 1 0	[84027]
	137181.18	(0.05)	23 2 1 - 22 2 1	[84027]
	137182.58	(0.05)	23 0 0 - 22 0 0	[84027]
	155027.73	(0.05)	26 0 3 - 25 0 3	[84027]
	155030.13	(0.05)	26 8 2 - 25 8 2	[84027]
	155030.81	(0.05)	26 9 3 - 25 9 3	[84027]
	155033.93	(0.05)	26 5 0 - 25 5 0	[84027]
	155033.93	(0.05)	26 6 5 - 25 6 5	[84027]
	155035.17	(0.05)	26 3 4 - 25 3 4	[84027]
	155035.17	(0.05)	26 9 5 - 25 9 5	[84027]
	155039.27	(0.05)	26 3 -1 - 25 3 -1	[84027]
	155040.14	(0.05)	26 1 3 - 25 1 3	[84027]
	155041.46	(0.05)	26 1 -2 - 25 1 -2	[84027]
	155042.47	(0.05)	26 8 3 - 25 8 3	[84027]
	155043.40	(0.05)	26 4 4 - 25 4 4	[84027]
	155043.40	(0.05)	26 7 2 - 25 7 2	[84027]
	155047.22	(0.05)	26 7 4 - 25 7 4	[84027]
	155048.19	(0.05)	26 5 4 - 25 5 4	[84027]
	155049.37	(0.05)	26 2 3 - 25 2 3	[84027]
	155049.37	(0.05)	26 4 0 - 25 4 0	[84027]
	155051.13	(0.05)	26 2 -1 - 25 2 -1	[84027]
	155051.13	(0.05)	26 7 3 - 25 7 3	[84027]

TABLE 19.2. Microwave spectrum of 2-butyne-1,1,1-d₃ — ContinuedC₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'K'm'_H - J''K''m''_H$	Ref.
	155052.02	(0.05)	26 0 2 - 25 0 2	[84027]
	155052.74	(0.05)	26 5 1 - 25 5 1	[84027]
	155053.70	(0.05)	26 6 2 - 25 6 2	[84027]
	155055.51	(0.05)	26 3 3 - 25 3 3	[84027]
	155057.03	(0.05)	26 6 3 - 25 6 3	[84027]
	155057.70	(0.05)	26 4 3 - 25 4 3	[84027]
	155058.77	(0.05)	26 1 2 - 25 1 2	[84027]
	155058.77	(0.05)	26 3 0 - 25 3 0	[84027]
	155059.87	(0.05)	26 5 3 - 25 5 3	[84027]
	155060.97	(0.05)	26 5 2 - 25 5 2	[84027]
	155061.57	(0.05)	26 4 1 - 25 4 1	[84027]
	155062.06	(0.05)	26 1-1 - 25 1-1	[84027]
	155065.41	(0.05)	26 2 2 - 25 2 2	[84027]
	155065.41	(0.05)	26 4 2 - 25 4 2	[84027]
	155066.10	(0.05)	26 2 0 - 25 2 0	[84027]
	155066.79	(0.05)	26 3 2 - 25 3 2	[84027]
	155067.41	(0.05)	26 0 1 - 25 0 1	[84027]
	155067.41	(0.05)	26 3 1 - 25 3 1	[84027]
	155070.43	(0.05)	26 1 0 - 25 1 0	[84027]
	155070.43	(0.05)	26 1 1 - 25 1 1	[84027]
	155070.43	(0.05)	26 2 1 - 25 2 1	[84027]
	155072.03	(0.05)	26 0 0 - 25 0 0	[84027]

Table 20.1. Molecular constants for 1-butyne (C_4H_6) in the ground and lowest torsional and bending states.

Parameter	Ground State	$v_{24} = 1$ Methyl torsion	$v_{15} = 1$ C≡C-C bend
<u>Rotational Constants</u> [present]			
A'' (MHz)	27147.8126(50)	28014.44(97)	26407.94(25)
B'' (MHz)	4546.47932(83)	4544.7101(82)	4559.084(8)
C'' (MHz)	4086.87510(80)	4086.3148(95)	4092.689(4)
τ_1 (MHz)	0.150285(16)	0.2328(30)	0.0786(13)
τ_2 (MHz)	0.0118211(46)	0.02317(52)	$-0.69(170) \times 10^{-4}$
τ_3^a (MHz)	1.019(1)	1.31(12)	0.077(26)
τ_{aaaa} (MHz)	-2.147587(584)	-2.75(354)	3.71(78)
τ_{bbbb} (MHz)	-0.0160141(43)	-0.015469(83)	-0.015969(65)
τ_{cccc} (MHz)	-0.0059185(41)	-0.00426(38)	-0.005428(16)
H_J (Hz)	0.00933(36)		
H_{JK} (Hz)	-0.3410(280)		-4.84(41)
H_{KJ} (Hz)	-0.6504(933)		
H_K (Hz)	33.55(130)		
h_J (Hz)	0.00681(22)		
h_{JK} (Hz)	0.1754(238)		
h_K (Hz)	-15.68(196)		
<u>Internal Rotation Constants</u> [85014, 83039]			
ω_1 (s)	$-0.1469(12) \times 10^{-5}$		
$\theta(a,i)$	47.55(19) $^\circ$	48.454(13) $^\circ$	
I_α ($u \text{ \AA}^2$)	3.180(12)	3.1635 ^b	
s	82.81(8)	86.57(26)	
F (GHz)	175.30(66)	176.162	
V_3 (cm^{-1})	1089.9(53)	1144.8(4)	
<u>Electric Dipole Moment</u> [83038]			
μ_a (D)	0.763(3)		
μ_b (D)	0.170(4)		

^aThe value of τ_3 is fixed by setting $R_6 = 0$.

^bAssumed value.

Table 20.2. Molecular constants for the vibrationally excited states $v_{15} = 2$ and 3 and $v_{14} = 1$ of 1-butyne. [83038]

Vibrational State	A (MHz)	B (MHz)	C (MHz)	D_{JK} (kHz)
$v_{15} = 2$	25728.(39)	4571.424(23)	4098.195(23)	-8.8(21)
$v_{15} = 3$	25000.(32)	4583.534(26)	4103.500(29)	21.2(25)
$v_{14} = 1$	26991.(38)	4547.096(23)	4091.436(23)	-45.6(22)

Comments: For the $v_{2a}=1$ state the following transitions were not included in the fit:

Transition	Frequency (MHz)	$\Delta v(\text{obs-calc})$ (MHz)
$18_{2,17}-17_{2,16}$	154299.32	-0.58
$18_{3,15}-17_{3,14}$	156595.53	0.26
$18_{1,17}-17_{1,16}$	157387.87	0.14

and similarly for the $v_{15}=1$ state:

$4_{13} - 4_{04}$	24504.22	-2.02
$27_{3,24}-27_{3,25}$	30421.88	-4.35
$17_{6,12}-16_{6,11}$	147247.37	-0.82
$17_{5,13}-16_{5,12}$	147316.53	-0.40
$18_{5,14}-17_{5,13}$	156006.17	-0.56
$25_{1,24}-24_{1,23}$	215354.31	-0.45
$25_{3,23}-24_{3,22}$	216453.67	+0.93
$27_{1,26}-26_{1,25}$	231539.29	-1.02

TABLE 20.3. Microwave spectrum of 1-butyne

C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_1	Sym.	Vib. state	Ref.
CH ₃ CH ₂ CCH	8378.740	(0.010)	32(7,26) - 33(6,27)	0	E		[85014]
	8378.862	(0.010)	32(7,26) - 33(6,27)	0	A		[85014]
	8466.011	(0.010)	32(7,25) - 33(6,28)	0	E		[85014]
	8466.081	(0.010)	32(7,25) - 33(6,28)	0	A		[85014]
	8597.043	(0.010)	8(1, 7) - 7(2, 6)	0	A		[85014]
	8597.093	(0.010)	8(1, 7) - 7(2, 6)	0	E		[85014]
	8633.419	(0.010)	1(0, 1) - 0(0, 0)	0	E		[85014]
	8633.419	(0.010)	1(0, 1) - 0(0, 0)	0	A		[85014]
	8704.757	(0.010)	13(2,11) - 13(2,12)	0	E		[85014]
	8704.778	(0.010)	13(2,11) - 13(2,12)	0	A		[85014]
	8778.098	(0.010)	7(2, 5) - 8(1, 8)	0	E		[85014]
	8778.182	(0.010)	7(2, 5) - 8(1, 8)	0	A		[85014]
	9533.726	(0.010)	35(6,30) - 34(7,27)	0	A		[85014]
	9533.801	(0.010)	35(6,30) - 34(7,27)	0	E		[85014]
	9545.926	(0.010)	19(3,16) - 18(4,15)	0	A		[85014]
	9546.030	(0.010)	19(3,16) - 18(4,15)	0	E		[85014]
	9644.014	(0.010)	6(1, 5) - 6(1, 6)	0	E		[85014]
	9644.014	(0.010)	6(1, 5) - 6(1, 6)	0	A		[85014]
	9707.115	(0.010)	35(6,29) - 34(7,28)	0	A		[85014]
	9707.209	(0.010)	35(6,29) - 34(7,28)	0	E		[85014]
	9732.268	(0.010)	31(4,27) - 30(4,28)	0	E		[85014]
	9732.298	(0.010)	31(4,27) - 30(4,28)	0	A		[85014]
	9815.607	(0.010)	16(4,13) - 17(3,14)	0	E		[85014]
	9815.726	(0.010)	16(4,13) - 17(3,14)	0	A		[85014]
	9980.311	(0.010)	22(3,19) - 22(3,20)	0	E		[85014]
	9980.337	(0.010)	22(3,19) - 22(3,20)	0	A		[85014]
	10585.075	(0.010)	37(8,30) - 38(7,31)	0	E		[85014]
	10585.209	(0.010)	37(8,30) - 38(7,31)	0	A		[85014]
	10608.173	(0.010)	37(8,29) - 38(7,32)	0	E		[85014]
	10608.173	(0.010)	37(8,29) - 38(7,32)	0	A		[85014]
	10647.743	(0.010)	15(2,14) - 14(3,11)	0	A		[85014]
	10647.852	(0.010)	15(2,14) - 14(3,11)	0	E		[85014]
	11334.829	(0.010)	14(2,12) - 14(2,13)	0	E		[85014]
	11334.851	(0.010)	14(2,12) - 14(2,13)	0	A		[85014]
	11559.633	(0.010)	30(5,26) - 29(6,23)	0	A		[85014]
	11559.735	(0.010)	30(5,26) - 29(6,23)	0	E		[85014]
	11656.016	(0.010)	12(1,12) - 11(2, 9)	0	A		[85014]
	11656.122	(0.010)	12(1,12) - 11(2, 9)	0	E		[85014]
	11951.037	(0.010)	5(2, 4) - 6(1, 5)	0	E		[85014]
	11951.100	(0.010)	5(2, 4) - 6(1, 5)	0	A		[85014]
	12148.512	(0.010)	32(4,28) - 32(4,29)	0	E		[85014]
	12148.545	(0.010)	32(4,28) - 32(4,29)	0	A		[85014]
	12179.704	(0.010)	30(5,25) - 29(6,24)	0	A		[85014]
	12179.811	(0.010)	30(5,25) - 29(6,24)	0	E		[85014]
	12280.437	(0.010)	16(4,12) - 17(3,15)	0	E		[85014]
	12280.560	(0.010)	16(4,12) - 17(3,15)	0	A		[85014]
	12392.817	(0.010)	11(3, 8) - 12(2,11)	0	E		[85014]
	12392.918	(0.010)	11(3, 8) - 12(2,11)	0	A		[85014]
	17814.934	(0.010)	16(2,15) - 15(3,12)	0	A		[85014]
	17815.038	(0.010)	16(2,15) - 15(3,12)	0	E		[85014]
	17993.857	(0.010)	16(2,14) - 16(2,15)	0	E		[85014]
	17993.903	(0.010)	16(2,14) - 16(2,15)	0	A		[85014]
	18277.470	(0.010)	14(1,14) - 13(2,11)	0	A		[85014]
	18277.587	(0.010)	14(1,14) - 13(2,11)	0	E		[85014]
	18322.023	(0.010)	34(4,30) - 34(4,31)	0	E		[85014]
	18322.080	(0.010)	34(4,30) - 34(4,31)	0	A		[85014]
	18578.509	(0.010)	36(6,31) - 35(7,28)	0	A		[85014]
	18578.587	(0.010)	36(6,31) - 35(7,28)	0	E		[85014]
	18819.114	(0.010)	36(6,30) - 35(7,29)	0	A		[85014]
	18819.196	(0.010)	36(6,30) - 35(7,29)	0	E		[85014]
	19161.649	(0.010)	9(1, 8) - 8(2, 7)	0	A		[85014]
	19161.699	(0.010)	9(1, 8) - 8(2, 7)	0	E		[85014]
	19203.422	(0.010)	15(4,12) - 16(3,13)	0	E		[85014]
	19203.541	(0.010)	15(4,12) - 16(3,13)	0	A		[85014]
	19246.242	(0.010)	21(1,21) - 20(2,18)	0	A		[85014]
	19246.446	(0.010)	21(1,21) - 20(2,18)	0	E		[85014]
	19274.586	(0.010)	25(3,22) - 25(3,23)	0	E		[85014]

TABLE 20.3. Microwave spectrum of 1-butyne — Continued

C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$	$- J''(K_{-1}, K_{+1})$	ν_1	Sym.	Vib. state	Ref.
	19274.638	(0.010)	25(3,22)	- 25(3,23)	0	A		[85014]
	19525.595	(0.010)	36(8,29)	- 37(7,30)	0	E		[85014]
	19525.765	(0.010)	36(8,29)	- 37(7,30)	0	A		[85014]
	19541.712	(0.010)	36(8,28)	- 37(7,31)	0	E		[85014]
	19541.712	(0.010)	36(8,28)	- 37(7,31)	0	A		[85014]
	19580.715	(0.010)	20(3,17)	- 19(4,16)	0	A		[85014]
	19580.814	(0.010)	20(3,17)	- 19(4,16)	0	E		[85014]
	20460.103	(0.010)	10(3, 7)	- 11(2,10)	0	E		[85014]
	20460.211	(0.010)	10(3, 7)	- 11(2,10)	0	A		[85014]
	20559.226	(0.010)	15(1,15)	- 14(2,12)	0	A		[85014]
	20559.362	(0.010)	15(1,15)	- 14(2,12)	0	E		[85014]
	20590.394	(0.010)	31(5,27)	- 30(6,24)	0	A		[85014]
	20590.491	(0.010)	31(5,27)	- 30(6,24)	0	E		[85014]
	20611.922	(0.010)	9(1, 8)	- 9(1, 9)	0	E		[85014]
	20611.955	(0.010)	9(1, 8)	- 9(1, 9)	0	A		[85014]
	20941.642	(0.010)	15(4,11)	- 16(3,14)	0	E		[85014]
	20941.763	(0.010)	15(4,11)	- 16(3,14)	0	A		[85014]
	21213.563	(0.010)	20(1,20)	- 19(2,17)	0	A		[85014]
	21213.772	(0.010)	20(1,20)	- 19(2,17)	0	E		[85014]
	21441.066	(0.010)	31(5,26)	- 30(6,25)	0	A		[85014]
	21441.171	(0.010)	31(5,26)	- 30(6,25)	0	E		[85014]
	21752.955	(0.010)	21(3,19)	- 20(4,16)	0	A		[85014]
	21753.070	(0.010)	21(3,19)	- 20(4,16)	0	E		[85014]
	21837.181	(0.010)	5(2, 3)	- 6(1, 6)	0	E		[85014]
	21837.266	(0.010)	5(2, 3)	- 6(1, 6)	0	A		[85014]
	21889.923	(0.010)	20(5,16)	- 21(4,17)	0	E		[85014]
	21890.059	(0.010)	20(5,16)	- 21(4,17)	0	A		[85014]
	21918.565	(0.010)	4(2, 3)	- 5(1, 4)	0	E		[85014]
	21918.628	(0.010)	4(2, 3)	- 5(1, 4)	0	A		[85014]
	21991.115	(0.010)	26(4,23)	- 25(5,20)	0	A		[85014]
	21991.229	(0.010)	26(4,23)	- 25(5,20)	0	E		[85014]
	22043.809	(0.010)	17(2,15)	- 17(2,16)	0	E		[85014]
	22043.862	(0.010)	17(2,15)	- 17(2,16)	0	A		[85014]
	22127.227	(0.010)	16(1,16)	- 15(2,13)	0	A		[85014]
	22127.380	(0.010)	16(1,16)	- 15(2,13)	0	E		[85014]
	22149.020	(0.010)	35(4,31)	- 35(4,32)	0	E		[85014]
	22149.084	(0.010)	35(4,31)	- 35(4,32)	0	A		[85014]
	22407.987	(0.010)	5(0, 5)	- 4(1, 4)	0	A		[85014]
	22407.987	(0.010)	5(0, 5)	- 4(1, 4)	0	E		[85014]
	22428.630	(0.010)	20(5,15)	- 21(4,18)	0	E		[85014]
	22428.752	(0.010)	20(5,15)	- 21(4,18)	0	A		[85014]
	22503.813	(0.010)	19(1,19)	- 18(2,16)	0	A		[85014]
	22503.989	(0.010)	19(1,19)	- 18(2,16)	0	E		[85014]
	22972.558	(0.010)	17(1,17)	- 16(2,14)	0	A		[85014]
	22972.709	(0.010)	17(1,17)	- 16(2,14)	0	E		[85014]
	23060.375	(0.010)	1(1, 0)	- 1(0, 1)	0	A		[85014]
	23060.399	(0.010)	1(1, 0)	- 1(0, 1)	0	E		[85014]
	23095.302	(0.010)	18(1,18)	- 17(2,15)	0	A		[85014]
	23095.476	(0.010)	18(1,18)	- 17(2,15)	0	E		[85014]
	23148.910	(0.100)	17(2,15)	- 17(2,16)			1 ν_{15}	[83038]
	23357.735	(0.010)	26(3,23)	- 26(3,24)	0	E		[85014]
	23357.798	(0.010)	26(3,23)	- 26(3,24)	0	A		[85014]
	23514.680	(0.100)	3(1, 2)	- 3(0, 3)			1 ν_{15}	[83038]
	23527.086	(0.010)	2(1, 1)	- 2(0, 2)	0	E		[85014]
	23527.111	(0.010)	2(1, 1)	- 2(0, 2)	0	A		[85014]
	24162.217	(0.010)	25(6,20)	- 26(5,21)	0	E		[85014]
	24162.365	(0.010)	25(6,20)	- 26(5,21)	0	A		[85014]
	24240.063	(0.010)	3(1, 2)	- 3(0, 3)	0	E		[85014]
	24240.086	(0.010)	3(1, 2)	- 3(0, 3)	0	A		[85014]
	24316.393	(0.010)	26(6,19)	- 26(5,22)	0	E		[85014]
	24316.490	(0.010)	26(6,19)	- 26(5,22)	0	A		[85014]
	24504.220	(0.100)	4(1, 3)	- 4(0, 4)			1 ν_{15}	[83038]
	24652.929	(0.010)	17(2,16)	- 16(3,13)	0	A		[85014]
	24653.034	(0.010)	17(2,16)	- 16(3,13)	0	E		[85014]
	24786.453	(0.010)	26(4,22)	- 25(5,21)	0	A		[85014]
	24786.561	(0.010)	26(4,22)	- 25(5,21)	0	E		[85014]
	25092.47	(0.10)	10(1, 9)	- 10(1,10)	1	A		[83038]

TABLE 20.3. Microwave spectrum of 1-butyne — Continued

C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_1	Sym.	Vib. state	Ref.
	25094.50	(0.10)	10(1, 9) - 10(1,10)	1	<i>E</i>		[83038]
	25103.21	(0.10)	3(1, 2) - 3(0, 3)	1	<i>A</i>		[83038]
	25104.54	(0.10)	3(1, 2) - 3(0, 3)	1	<i>E</i>		[83038]
	25151.704	(0.010)	10(1, 9) - 10(1,10)	0	<i>A</i>		[85014]
	25151.704	(0.010)	10(1, 9) - 10(1,10)	0	<i>E</i>		[85014]
	25201.98	(0.10)	3(1, 3) - 2(1, 2)	1	<i>A</i>		[83038]
	25206.638	(0.010)	3(1, 3) - 2(1, 2)	0	<i>E</i>		[85014]
	25206.638	(0.010)	3(1, 3) - 2(1, 2)	0	<i>A</i>		[85014]
	25214.664	(0.010)	4(1, 3) - 4(0, 4)	0	<i>A</i>		[85014]
	25214.689	(0.010)	4(1, 3) - 4(0, 4)	0	<i>E</i>		[85014]
	25228.08	(0.10)	3(1, 3) - 2(1, 2)			1 ν_{14}	[83038]
	25251.160	(0.100)	3(1, 3) - 2(1, 2)			1 ν_{15}	[83038]
	25287.038	(0.010)	9(3, 7) - 10(2, 8)	0	<i>E</i>		[85014]
	25287.144	(0.010)	9(3, 7) - 10(2, 8)	0	<i>A</i>		[85014]
	25294.04	(0.10)	3(1, 3) - 2(1, 2)			2 ν_{15}	[83038]
	25394.410	(0.100)	42(7,36) - 41(8,33)				[83038]
	25484.010	(0.100)	42(7,35) - 41(8,34)				[83038]
	25785.31	(0.10)	18(2,16) - 18(2,17)	1	<i>A</i>		[83038]
	25786.130	(0.100)	5(1, 4) - 5(0, 5)			1 ν_{15}	[83038]
	25787.80	(0.10)	18(2,16) - 18(2,17)	1	<i>E</i>		[83038]
	25863.003	(0.010)	15(2,13) - 14(3,12)	0	<i>A</i>		[85014]
	25863.076	(0.010)	15(2,13) - 14(3,12)	0	<i>E</i>		[85014]
	25866.62	(0.10)	3(0, 3) - 2(0, 2)	1	<i>A</i>		[83038]
	25872.27	(0.01)	3(0, 3) - 2(0, 2)	0	<i>A</i>		[85014]
	25872.27	(0.01)	3(0, 3) - 2(0, 2)	0	<i>E</i>		[85014]
	25887.87	(0.10)	3(0, 3) - 2(0, 2)			1 ν_{14}	[83038]
	25894.74	(0.10)	3(2, 2) - 2(2, 1)	1	<i>A</i>		[83038]
	25899.58	(0.10)	3(2, 2) - 2(2, 1)	1	<i>E</i>		[83038]
	25901.108	(0.010)	3(2, 2) - 2(2, 1)	0	<i>A</i>		[85014]
	25901.108	(0.010)	3(2, 2) - 2(2, 1)	0	<i>E</i>		[85014]
	25916.50	(0.10)	3(2, 1) - 2(2, 0)	1	<i>E</i>		[83038]
	25916.50	(0.10)	3(2, 2) - 2(2, 1)			1 ν_{14}	[83038]
	25921.23	(0.10)	3(2, 1) - 2(2, 0)	1	<i>A</i>		[83038]
	25925.510	(0.100)	3(0, 3) - 2(0, 2)			1 ν_{15}	[83038]
	25928.839	(0.010)	3(2, 1) - 2(2, 0)	0	<i>A</i>		[85014]
	25928.839	(0.010)	3(2, 1) - 2(2, 0)	0	<i>E</i>		[85014]
	25943.75	(0.10)	3(2, 1) - 2(2, 0)			1 ν_{14}	[83038]
	25955.760	(0.100)	3(2, 2) - 2(2, 1)			1 ν_{15}	[83038]
	25977.23	(0.10)	3(0, 3) - 2(0, 2)			2 ν_{15}	[83038]
	25985.210	(0.100)	3(2, 1) - 2(2, 0)			1 ν_{15}	[83038]
	26008.77	(0.10)	3(2, 2) - 2(2, 1)			2 ν_{15}	[83038]
	26027.37	(0.10)	3(0, 3) - 2(0, 2)			3 ν_{15}	[83038]
	26040.22	(0.10)	3(2, 1) - 2(2, 0)			2 ν_{15}	[83038]
	26060.32	(0.10)	3(2, 2) - 2(2, 1)			3 ν_{15}	[83038]
	26073.17	(0.10)	4(1, 3) - 4(0, 4)	1	<i>A</i>		[83038]
	26074.63	(0.10)	4(1, 3) - 4(0, 4)	1	<i>E</i>		[83038]
	26093.72	(0.10)	3(2, 1) - 2(2, 0)			3 ν_{15}	[83038]
	26260.04	(0.10)	27(3,24) - 27(3,25)	1	<i>A</i>		[83038]
	26262.86	(0.10)	27(3,24) - 27(3,25)	1	<i>E</i>		[83038]
	26309.129	(0.010)	30(7,24) - 31(6,25)	0	<i>E</i>		[85014]
	26309.321	(0.010)	30(7,24) - 31(6,25)	0	<i>A</i>		[85014]
	26351.178	(0.010)	30(7,23) - 31(6,26)	0	<i>A</i>		[85014]
	26351.178	(0.010)	30(7,23) - 31(6,26)	0	<i>E</i>		[85014]
	26471.062	(0.010)	5(1, 4) - 5(0, 5)	0	<i>A</i>		[85014]
	26471.062	(0.010)	5(1, 4) - 5(0, 5)	0	<i>E</i>		[85014]
	26505.694	(0.010)	36(4,32) - 36(4,33)	0	<i>E</i>		[85014]
	26505.775	(0.010)	36(4,32) - 36(4,33)	0	<i>A</i>		[85014]
	26576.070	(0.100)	18(2,16) - 18(2,17)				[83038]
	26576.93	(0.10)	3(1, 2) - 2(1, 1)	1	<i>A</i>		[83038]
	26585.250	(0.100)	3(1, 2) - 2(1, 1)				[83038]
	26594.70	(0.10)	3(1, 2) - 2(1, 1)			1 ν_{14}	[83038]
	26713.46	(0.10)	3(1, 2) - 2(1, 1)			2 ν_{15}	[83038]
	26775.32	(0.10)	3(1, 2) - 2(1, 1)			3 ν_{15}	[83038]
	27322.16	(0.10)	5(1, 4) - 5(0, 5)	1	<i>A</i>		[83038]
	27323.68	(0.10)	5(1, 4) - 5(0, 5)	1	<i>E</i>		[83038]
	27380.260	(0.100)	6(1, 5) - 6(0, 6)			1 ν_{15}	[83038]
	27653.560	(0.100)	37(6,32) - 36(7,29)				[83038]

TABLE 20.3. Microwave spectrum of 1-butyne — Continued

C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$	-	$J''(K_{-1}, K_{+1})$	ν_1	Sym.	Vib. state	Ref.
	27810.580	(0.100)	46(5,41)	-	46(5,42)				[83038]
	27852.890	(0.100)	18(2,16)	-	18(2,17)			1 ν_{15}	[83038]
	27959.250	(0.100)	27(3,24)	-	27(3,25)				[83038]
	27984.060	(0.100)	37(6,31)	-	36(7,30)				[83038]
	28033.410	(0.100)	6(1, 5)	-	6(0, 6)				[83038]
	28434.520	(0.100)	14(4,11)	-	15(3,12)				[83038]
	28439.730	(0.100)	35(8,28)	-	36(7,29)				[83038]
	28450.790	(0.100)	35(8,27)	-	36(7,30)				[83038]
	28667.580	(0.100)	9(3, 6)	-	10(2, 9)				[83038]
	28873.53	(0.10)	6(1, 5)	-	6(0, 6)	1	A		[83038]
	28875.22	(0.10)	6(1, 5)	-	6(0, 6)	1	E		[83038]
	29318.030	(0.100)	7(1, 6)	-	7(0, 7)			1 ν_{15}	[83038]
	29630.800	(0.100)	14(4,10)	-	15(3,13)				[83038]
	29640.910	(0.100)	32(5,28)	-	31(6,25)				[83038]
	29891.530	(0.100)	21(3,18)	-	20(4,17)				[83038]
	29929.810	(0.100)	7(1, 6)	-	7(0, 7)				[83038]
	29998.250	(0.100)	22(3,20)	-	21(4,17)				[83038]
	30117.500	(0.100)	11(1,10)	-	11(1,11)				[83038]
	30421.880	(0.100)	27(3,24)	-	27(3,25)			1 ν_{15}	[83038]
	30592.800	(0.100)	40(9,32)	-	41(8,33)				[83038]
	30595.400	(0.100)	40(9,31)	-	41(8,34)				[83038]
	30754.33	(0.10)	7(1, 6)	-	7(0, 7)	1	A		[83038]
	30756.20	(0.10)	7(1, 6)	-	7(0, 7)	1	E		[83038]
	30794.720	(0.100)	32(5,27)	-	31(6,26)				[83038]
	30846.620	(0.100)	27(4,24)	-	26(5,21)				[83038]
	30918.670	(0.100)	19(5,15)	-	20(4,16)				[83038]
	31112.700	(0.100)	18(2,17)	-	17(3,14)				[83038]
	31156.31	(0.10)	28(3,25)	-	28(3,26)	1	A		[83038]
	31159.56	(0.10)	28(3,25)	-	28(3,26)	1	E		[83038]
	31286.920	(0.100)	19(5,14)	-	20(4,17)				[83038]
	31409.710	(0.100)	37(4,33)	-	37(4,34)				[83038]
	31584.840	(0.100)	19(2,17)	-	19(2,18)				[83038]
	31630.530	(0.100)	8(1, 7)	-	8(0, 8)			1 ν_{15}	[83038]
	31977.240	(0.100)	6(0, 6)	-	5(1, 5)				[83038]
	32190.130	(0.100)	8(1, 7)	-	8(0, 8)				[83038]
	32993.63	(0.10)	8(1, 7)	-	8(0, 8)	1	A		[83038]
	32995.70	(0.10)	8(1, 7)	-	8(0, 8)	1	E		[83038]
	33594.88	(0.10)	4(1, 4)	-	3(1, 3)	1	A		[83038]
	33600.660	(0.100)	4(1, 4)	-	3(1, 3)				[83038]
	33629.22	(0.10)	4(1, 4)	-	3(1, 3)			1 ν_{14}	[83038]
	33659.450	(0.100)	4(1, 4)	-	3(1, 3)			1 ν_{15}	[83038]
	33716.21	(0.10)	4(1, 4)	-	3(1, 3)			3 ν_{15}	[83038]
	33771.04	(0.10)	4(1, 4)	-	3(1, 3)			2 ν_{15}	[83038]
	34349.540	(0.100)	9(1, 8)	-	9(0, 9)			1 ν_{15}	[83038]
	34457.64	(0.10)	4(0, 4)	-	3(0, 3)	1	A		[83038]
	34463.650	(0.100)	4(0, 4)	-	3(0, 3)				[83038]
	34520.88	(0.10)	4(2, 3)	-	3(2, 2)	1	A		[83038]
	34528.910	(0.100)	4(2, 3)	-	3(2, 2)				[83038]
	34532.920	(0.100)	4(0, 4)	-	3(0, 3)			1 ν_{15}	[83038]
	34550.310	(0.100)	4(3, 1)	-	3(3, 0)				[83038]
	34550.310	(0.100)	4(3, 2)	-	3(3, 1)				[83038]
	34566.690	(0.100)	27(4,23)	-	26(5,22)				[83038]
	34570.45	(0.10)	4(3, 1)	-	3(3, 0)			1 ν_{14}	[83038]
	34570.45	(0.10)	4(3, 2)	-	3(3, 1)			1 ν_{14}	[83038]
	34587.15	(0.10)	4(2, 2)	-	3(2, 1)	1	A		[83038]
	34598.200	(0.100)	4(2, 2)	-	3(2, 1)				[83038]
	34601.460	(0.100)	4(2, 3)	-	3(2, 2)			1 ν_{15}	[83038]
	34618.01	(0.10)	4(2, 2)	-	3(2, 1)			1 ν_{14}	[83038]
	34671.86	(0.10)	4(2, 3)	-	3(2, 2)			2 ν_{15}	[83038]
	34675.240	(0.100)	4(2, 2)	-	3(2, 1)			1 ν_{15}	[83038]
	34694.12	(0.10)	4(3, 1)	-	3(3, 0)			2 ν_{15}	[83038]
	34694.12	(0.10)	4(3, 2)	-	3(3, 1)			2 ν_{15}	[83038]
	34740.11	(0.10)	4(2, 3)	-	3(2, 2)			3 ν_{15}	[83038]
	34750.26	(0.10)	4(2, 2)	-	3(2, 1)			2 ν_{15}	[83038]
	34762.66	(0.10)	4(3, 1)	-	3(3, 0)			3 ν_{15}	[83038]
	34762.66	(0.10)	4(3, 2)	-	3(3, 1)			3 ν_{15}	[83038]
	34823.74	(0.10)	4(2, 2)	-	3(2, 1)			3 ν_{15}	[83038]

TABLE 20.3. Microwave spectrum of 1-butyne — Continued

C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_1	Sym.	Vib. state	Ref.
	34844.610	(0.100)	9(1, 8) - 9(0, 9)				[83038]
	35224.610	(0.100)	29(7,23) - 30(6,24)				[83038]
	35253.330	(0.100)	29(7,22) - 30(6,25)				[83038]
	35427.69	(0.10)	4(1, 3) - 3(1, 2)	1	A		[83038]
	35438.280	(0.100)	4(1, 3) - 3(1, 2)				[83038]
	35450.97	(0.10)	4(1, 3) - 3(1, 2)			1 ν_{14}	[83038]
	35495.960	(0.100)	12(1,11) - 12(1,12)				[83038]
	35524.240	(0.100)	4(1, 3) - 3(1, 2)			1 ν_{15}	[83038]
	35608.06	(0.10)	4(1, 3) - 3(1, 2)			2 ν_{15}	[83038]
	35623.10	(0.10)	9(1, 8) - 9(0, 9)	1	E		[83038]
	35690.12	(0.10)	4(1, 3) - 3(1, 2)			3 ν_{15}	[83038]
	37922.130	(0.100)	10(1, 9) - 10(0,10)				[83038]
	41116.730	(0.100)	11(1,10) - 11(0,11)			1 ν_{15}	[83038]
	41268.650	(0.100)	13(1,12) - 13(1,13)				[83038]
	58729.06	(0.10)	7(1, 7) - 6(1, 6)	1	A		[83038]
	58736.270	(0.100)	7(1, 7) - 6(1, 6)				[83038]
	58835.160	(0.100)	7(1, 7) - 6(1, 6)			1 ν_{15}	[83038]
	60047.260	(0.100)	7(0, 7) - 6(0, 6)				[83038]
	60151.310	(0.100)	7(0, 7) - 6(0, 6)			1 ν_{15}	[83038]
	60378.970	(0.100)	7(2, 6) - 6(2, 5)				[83038]
	60489.710	(0.100)	7(3, 5) - 6(3, 4)				[83038]
	60497.830	(0.100)	7(3, 4) - 6(3, 3)				[83038]
	60734.25	(0.10)	7(2, 5) - 6(2, 4)	1	A		[83038]
	60762.110	(0.100)	7(2, 5) - 6(2, 4)				[83038]
	60910.300	(0.100)	7(2, 5) - 6(2, 4)			1 ν_{15}	[83038]
	61928.48	(0.10)	7(1, 6) - 6(1, 5)	1	A		[83038]
	61943.540	(0.100)	7(1, 6) - 6(1, 5)				[83038]
	62088.930	(0.100)	7(1, 6) - 6(1, 5)			1 ν_{15}	[83038]
	68492.750	(0.100)	8(0, 8) - 7(0, 7)				[83038]
	68498.34	(0.10)	8(0, 8) - 7(0, 7)	1	A		[83038]
	68603.700	(0.100)	8(0, 8) - 7(0, 7)			1 ν_{15}	[83038]
	68967.83	(0.10)	8(2, 7) - 7(2, 6)	1	A		[83038]
	68980.200	(0.100)	8(2, 7) - 7(2, 6)				[83038]
	69114.170	(0.100)	8(5, 3) - 7(5, 2)				[83038]
	69114.170	(0.100)	8(6, 2) - 7(6, 1)				[83038]
	69119.190	(0.100)	8(7, 1) - 7(7, 0)				[83038]
	69119.700	(0.100)	8(2, 7) - 7(2, 6)			1 ν_{15}	[83038]
	69122.250	(0.100)	8(4, 4) - 7(4, 3)				[83038]
	69122.250	(0.100)	8(4, 5) - 7(4, 4)				[83038]
	69143.550	(0.100)	8(3, 6) - 7(3, 5)				[83038]
	69159.960	(0.100)	8(3, 5) - 7(3, 4)				[83038]
	69255.960	(0.100)	8(5, 4) - 7(5, 3)			1 ν_{15}	[83038]
	69291.980	(0.100)	8(3, 6) - 7(3, 5)			1 ν_{15}	[83038]
	69310.390	(0.100)	8(3, 5) - 7(3, 4)			1 ν_{15}	[83038]
	69513.71	(0.10)	8(2, 6) - 7(2, 5)	1	A		[83038]
	69549.340	(0.100)	8(2, 6) - 7(2, 5)				[83038]
	70737.45	(0.10)	8(1, 7) - 7(1, 6)	1	A		[83038]
	70752.820	(0.100)	8(1, 7) - 7(1, 6)				[83038]
	70916.220	(0.100)	8(1, 7) - 7(1, 6)			1 ν_{15}	[83038]
	76902.60	(0.03)	9(0, 9) - 8(0, 8)	1	A		[83038]
	76902.872	(0.030)	9(0, 9) - 8(0, 8)	1	E		[83039]
	77559.224	(0.030)	9(2, 8) - 8(2, 7)	1	A		[83039]
	77559.529	(0.030)	9(2, 8) - 8(2, 7)	1	E		[83039]
	78329.277	(0.030)	9(2, 7) - 8(2, 6)	1	A		[83039]
	78329.625	(0.030)	9(2, 7) - 8(2, 6)	1	E		[83039]
	79529.90	(0.03)	9(1, 8) - 8(1, 7)	1	A		[83039]
	79530.365	(0.030)	9(1, 8) - 8(1, 7)	1	E		[83039]
	83776.900	(0.100)	10(1,10) - 9(1, 9)				[83038]
	83910.560	(0.100)	10(1,10) - 9(1, 9)			1 ν_{15}	[83038]
	85239.240	(0.100)	10(0,10) - 9(0, 9)				[83038]
	85259.624	(0.100)	10(0,10) - 9(0, 9)	1	A		[83038]
	85357.740	(0.100)	10(0,10) - 9(0, 9)			1 ν_{15}	[83038]
	86140.532	(0.100)	10(2, 9) - 9(2, 8)	1	A		[83038]
	86152.530	(0.100)	10(2, 9) - 9(2, 8)				[83038]
	86322.000	(0.100)	10(2, 9) - 9(2, 8)			1 ν_{15}	[83038]
	86462.570	(0.100)	10(3, 8) - 9(3, 7)				[83038]
	86513.840	(0.100)	10(3, 7) - 9(3, 6)				[83038]

TABLE 20.3. Microwave spectrum of 1-butyne — Continued

C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_1	Sym.	Vib. state	Ref.
	86649.190	(0.100)	10(3, 8) - 9(3, 7)			1 ν_{15}	[83038]
	86706.620	(0.100)	10(3, 7) - 9(3, 6)			1 ν_{15}	[83038]
	87181.866	(0.100)	10(2, 8) - 9(2, 7)	1	A		[83038]
	87235.840	(0.100)	10(2, 8) - 9(2, 7)				[83038]
	87470.670	(0.100)	10(2, 8) - 9(2, 7)			1 ν_{15}	[83038]
	88316.640	(0.100)	10(1, 9) - 9(1, 8)				[83038]
	88511.930	(0.100)	10(1, 9) - 9(1, 8)			1 ν_{15}	[83038]
	100406.52	(0.10)	12(1, 12) - 11(1, 11)	1	A		[83038]
	100407.980	(0.100)	12(1, 12) - 11(1, 11)				[83038]
	101796.690	(0.100)	12(0, 12) - 11(0, 11)				[83038]
	101834.76	(0.10)	12(0, 12) - 11(0, 11)	1	A		[83038]
	101917.550	(0.100)	12(0, 12) - 11(0, 11)			1 ν_{15}	[83038]
	103267.82	(0.10)	12(2, 11) - 11(2, 10)	1	A		[83038]
	103277.220	(0.100)	12(2, 11) - 11(2, 10)				[83038]
	103473.030	(0.100)	12(2, 11) - 11(2, 10)			1 ν_{15}	[83038]
	103721.80	(0.10)	12(4, 9) - 11(4, 8)	1	A		[83038]
	103724.70	(0.10)	12(4, 8) - 11(4, 7)	1	A		[83038]
	103725.400	(0.100)	12(10, 2) - 11(10, 1)				[83038]
	103884.44	(0.10)	12(3, 9) - 11(3, 8)	1	A		[83038]
	103900.887	(0.100)	12(6, 6) - 11(6, 5)			1 ν_{15}	[83038]
	103921.222	(0.100)	12(5, 8) - 11(5, 7)			1 ν_{15}	[83038]
	103921.740	(0.100)	12(3, 9) - 11(3, 8)				[83038]
	103966.458	(0.100)	12(4, 9) - 11(4, 8)			1 ν_{15}	[83038]
	103970.300	(0.100)	12(4, 8) - 11(4, 7)			1 ν_{15}	[83038]
	129630.240	(0.100)	15(7, 8) - 14(7, 7)				[83038]
	129631.300	(0.100)	15(8, 7) - 14(8, 6)				[83038]
	129641.280	(0.100)	15(9, 6) - 14(9, 5)				[83038]
	129642.540	(0.100)	15(6, 10) - 14(6, 9)				[83038]
	129657.700	(0.100)	15(10, 5) - 14(10, 4)				[83038]
	129756.720	(0.100)	15(4, 12) - 14(4, 11)				[83038]
	129768.260	(0.100)	15(14, 1) - 14(14, 0)				[83038]
	129772.620	(0.100)	15(4, 11) - 14(4, 10)				[83038]
	140352.810	(0.030)	16(1, 15) - 15(1, 14)	1	A		[83039]
	140353.470	(0.030)	16(1, 15) - 15(1, 14)	1	E		[83039]
	140825.594	(0.030)	16(2, 14) - 15(2, 13)	1	A		[83039]
	140826.375	(0.030)	16(2, 14) - 15(2, 13)	1	E		[83039]
	142767.540	(0.030)	17(0, 17) - 16(0, 16)			1 ν_{15}	[83039]
	146071.040	(0.030)	17(2, 16) - 16(2, 15)			1 ν_{15}	[83039]
	146923.496	(0.030)	17(8, 9) - 16(8, 8)				[83039]
	146928.455	(0.030)	17(7, 10) - 16(7, 9)				[83039]
	146930.570	(0.030)	17(9, 8) - 16(9, 7)				[83039]
	146946.235	(0.030)	17(10, 7) - 16(10, 6)				[83039]
	146952.248	(0.030)	17(6, 11) - 16(6, 10)				[83039]
	146968.434	(0.030)	17(11, 6) - 16(11, 5)				[83039]
	146996.121	(0.030)	17(12, 5) - 16(12, 4)				[83039]
	147009.169	(0.030)	17(5, 13) - 16(5, 12)				[83039]
	147010.193	(0.030)	17(5, 12) - 16(5, 11)				[83039]
	147120.281	(0.030)	17(4, 14) - 16(4, 13)				[83039]
	147122.558	(0.030)	17(3, 15) - 16(3, 14)				[83039]
	147158.755	(0.030)	17(4, 13) - 16(4, 12)				[83039]
	147247.370	(0.030)	17(6, 12) - 16(6, 11)			1 ν_{15}	[83039]
	147316.530	(0.030)	17(5, 13) - 16(5, 12)			1 ν_{15}	[83039]
	147318.280	(0.030)	17(5, 12) - 16(5, 11)			1 ν_{15}	[83039]
	147433.720	(0.030)	17(3, 15) - 16(3, 14)			1 ν_{15}	[83039]
	147440.050	(0.030)	17(4, 14) - 16(4, 13)			1 ν_{15}	[83039]
	147485.400	(0.030)	17(4, 13) - 16(4, 12)			1 ν_{15}	[83039]
	147739.790	(0.030)	17(3, 14) - 16(3, 13)	1	A		[83039]
	147740.350	(0.030)	17(3, 14) - 16(3, 13)	1	E		[83039]
	148214.020	(0.030)	17(3, 14) - 16(3, 13)			1 ν_{15}	[83039]
	148848.347	(0.030)	17(1, 16) - 16(1, 15)				[83039]
	149080.150	(0.030)	17(1, 16) - 16(1, 15)			1 ν_{15}	[83039]
	149786.230	(0.030)	17(2, 15) - 16(2, 14)	1	A		[83039]
	149787.060	(0.030)	17(2, 15) - 16(2, 14)	1	E		[83039]
	149875.734	(0.030)	17(2, 15) - 16(2, 14)				[83039]
	149998.449	(0.030)	18(1, 18) - 17(1, 17)				[83039]
	150203.210	(0.030)	18(1, 18) - 17(1, 17)			1 ν_{15}	[83039]
	150286.440	(0.030)	17(2, 15) - 16(2, 14)			1 ν_{15}	[83039]

TABLE 20.3. Microwave spectrum of 1-butyne — Continued

C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_1	Sym.	Vib. state	Ref.
	150748.243	(0.030)	18(0,18) - 17(0,17)				[83039]
	150898.790	(0.030)	18(0,18) - 17(0,17)			1 ν_{15}	[83039]
	154283.853	(0.030)	18(2,17) - 17(2,16)				[83039]
	154299.320	(0.030)	18(2,17) - 17(2,16)	1	A		[83039]
	154299.790	(0.030)	18(2,17) - 17(2,16)	1	E		[83039]
	154535.790	(0.030)	18(2,17) - 17(2,16)			1 ν_{15}	[83039]
	155570.723	(0.030)	18(8,11) - 17(8,10)				[83039]
	155575.754	(0.030)	18(9,10) - 17(9,9)				[83039]
	155579.536	(0.030)	18(7,12) - 17(7,11)				[83039]
	155590.560	(0.030)	18(10,9) - 17(10,8)				[83039]
	155610.315	(0.030)	18(6,13) - 17(6,12)				[83039]
	155612.770	(0.030)	18(11,8) - 17(11,7)				[83039]
	155641.151	(0.030)	18(12,7) - 17(12,6)				[83039]
	155674.641	(0.030)	18(13,6) - 17(13,5)				[83039]
	155679.954	(0.030)	18(5,14) - 17(5,13)				[83039]
	155681.729	(0.030)	18(5,13) - 17(5,12)				[83039]
	155712.785	(0.030)	18(14,5) - 17(14,4)				[83039]
	155748.470	(0.030)	18(3,16) - 17(3,15)	1	A		[83039]
	155749.020	(0.030)	18(3,16) - 17(3,15)	1	E		[83039]
	155755.123	(0.030)	18(15,4) - 17(15,3)				[83039]
	155777.656	(0.030)	18(3,16) - 17(3,15)				[83039]
	155801.449	(0.030)	18(16,3) - 17(16,2)				[83039]
	155808.730	(0.030)	18(4,15) - 17(4,14)				[83039]
	155851.507	(0.030)	18(17,2) - 17(17,1)				[83039]
	155866.079	(0.030)	18(4,14) - 17(4,13)				[83039]
	156006.170	(0.030)	18(5,14) - 17(5,13)			1 ν_{15}	[83039]
	156009.040	(0.030)	18(5,13) - 17(5,12)			1 ν_{15}	[83039]
	156103.500	(0.030)	18(3,16) - 17(3,15)			1 ν_{15}	[83039]
	156148.340	(0.030)	18(4,15) - 17(4,14)			1 ν_{15}	[83039]
	156215.920	(0.030)	18(4,14) - 17(4,13)			1 ν_{15}	[83039]
	156595.530	(0.030)	18(3,15) - 17(3,14)	1	A		[83039]
	156596.120	(0.030)	18(3,15) - 17(3,14)	1	E		[83039]
	156693.385	(0.030)	18(3,15) - 17(3,14)				[83039]
	157120.000	(0.030)	18(3,15) - 17(3,14)			1 ν_{15}	[83039]
	157324.525	(0.030)	18(1,17) - 17(1,16)				[83039]
	157387.870	(0.030)	18(1,17) - 17(1,16)	1	A		[83039]
	157388.560	(0.030)	18(1,17) - 17(1,16)	1	E		[83039]
	157548.810	(0.030)	18(1,17) - 17(1,16)			1 ν_{15}	[83039]
	158224.720	(0.030)	19(1,19) - 18(1,18)				[83039]
	158437.520	(0.030)	19(1,19) - 18(1,18)			1 ν_{15}	[83039]
	158731.400	(0.030)	18(2,16) - 17(2,15)	1	A		[83039]
	158732.260	(0.030)	18(2,16) - 17(2,15)	1	E		[83039]
	158816.208	(0.030)	18(2,16) - 17(2,15)				[83039]
	158867.902	(0.030)	19(0,19) - 18(0,18)				[83039]
	159028.960	(0.030)	19(0,19) - 18(0,18)			1 ν_{15}	[83039]
	159239.760	(0.030)	18(2,16) - 17(2,15)			1 ν_{15}	[83039]
	213039.730	(0.030)	25(2,24) - 24(2,23)	1	A		[83039]
	213040.220	(0.030)	25(2,24) - 24(2,23)	1	E		[83039]
	215354.310	(0.030)	25(1,24) - 24(1,23)			1 ν_{15}	[83039]
	215440.590	(0.030)	25(1,24) - 24(1,23)	1	A		[83039]
	215441.150	(0.030)	25(1,24) - 24(1,23)	1	E		[83039]
	215871.360	(0.030)	26(1,26) - 25(1,25)			1 ν_{15}	[83039]
	216023.720	(0.030)	26(0,26) - 25(0,25)			1 ν_{15}	[83039]
	216453.870	(0.030)	25(3,23) - 24(3,22)			1 ν_{15}	[83039]
	216995.440	(0.030)	25(5,20) - 24(5,19)			1 ν_{15}	[83039]
	217170.640	(0.030)	25(4,22) - 24(4,21)			1 ν_{15}	[83039]
	217795.510	(0.030)	25(4,21) - 24(4,20)			1 ν_{15}	[83039]
	220481.429	(0.030)	25(2,23) - 24(2,22)	1	A		[83039]
	220482.490	(0.030)	25(2,23) - 24(2,22)	1	E		[83039]
	223773.601	(0.030)	27(1,27) - 26(1,26)				[83039]
	223916.235	(0.030)	27(0,27) - 26(0,26)				[83039]
	224055.570	(0.030)	27(1,27) - 26(1,26)			1 ν_{15}	[83039]
	224178.440	(0.030)	27(0,27) - 26(0,26)			1 ν_{15}	[83039]
	229564.277	(0.030)	27(2,26) - 26(2,25)				[83039]
	231415.881	(0.030)	27(1,26) - 26(1,25)				[83039]
	231539.290	(0.030)	27(1,26) - 26(1,25)			1 ν_{15}	[83039]
	231944.949	(0.030)	28(1,28) - 27(1,27)				[83039]

TABLE 20.3. Microwave spectrum of 1-butyne — Continued

C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$	-	$J''(K_{-1}, K_{+1})$	ν_1	Sym.	Vib. state	Ref.
	232060.337	(0.030)	28(0,28)	-	27(0,27)				[83039]
	232236.290	(0.030)	28(1,28)	-	27(1,27)			1 ν_{15}	[83039]
	232334.990	(0.030)	28(0,28)	-	27(0,27)			1 ν_{15}	[83039]
	233148.469	(0.030)	27(3,25)	-	26(3,24)				[83039]
	233393.175	(0.030)	27(10,18)	-	26(10,17)				[83039]
	233400.855	(0.030)	27(9,19)	-	26(9,18)				[83039]
	233404.369	(0.030)	27(11,17)	-	26(11,16)				[83039]
	233430.205	(0.030)	27(12,16)	-	26(12,15)				[83039]
	233435.560	(0.030)	27(8,20)	-	26(8,19)				[83039]
	233467.477	(0.030)	27(13,15)	-	26(13,14)				[83039]
	233511.303	(0.030)	27(7,21)	-	26(7,20)				[83039]
	233514.305	(0.030)	27(14,14)	-	26(14,13)				[83039]
	233569.398	(0.030)	27(15,13)	-	26(15,12)				[83039]
	233631.992	(0.030)	27(16,12)	-	26(16,11)				[83039]
	233654.905	(0.030)	27(6,22)	-	26(6,21)				[83039]
	233657.794	(0.030)	27(6,21)	-	26(6,20)				[83039]
	233701.367	(0.030)	27(17,11)	-	26(17,10)				[83039]
	233776.852	(0.030)	27(18,10)	-	26(18,9)				[83039]
	233858.377	(0.030)	27(19,9)	-	26(19,8)				[83039]
	233902.235	(0.030)	27(5,23)	-	26(5,22)				[83039]
	233945.507	(0.030)	27(20,8)	-	26(20,7)				[83039]
	233968.988	(0.030)	27(5,22)	-	26(5,21)				[83039]
	234037.962	(0.030)	27(21,7)	-	26(21,6)				[83039]
	234097.584	(0.030)	27(4,24)	-	26(4,23)				[83039]
	234135.698	(0.030)	27(22,6)	-	26(22,5)				[83039]
	234238.360	(0.030)	27(23,5)	-	26(23,4)				[83039]
	234345.937	(0.030)	27(24,4)	-	26(24,3)				[83039]
	234458.414	(0.030)	27(25,3)	-	26(25,2)				[83039]
	234575.510	(0.030)	27(26,2)	-	26(26,1)				[83039]
	234974.328	(0.030)	27(4,23)	-	26(4,22)				[83039]
	237562.970	(0.030)	27(3,24)	-	26(3,23)	1	A		[83039]
	237564.080	(0.030)	27(3,24)	-	26(3,23)	1	E		[83039]
	237655.972	(0.030)	27(2,25)	-	26(2,24)				[83039]
	237735.300	(0.030)	27(2,25)	-	26(2,24)	1	A		[83039]
	237736.360	(0.030)	27(2,25)	-	26(2,24)	1	E		[83039]
	239488.394	(0.030)	28(1,27)	-	27(1,26)				[83039]
	304069.833	(0.030)	36(1,35)	-	35(1,34)				[83039]
	305371.868	(0.030)	37(1,37)	-	36(1,36)				[83039]
	305387.097	(0.030)	37(0,37)	-	36(0,36)				[83039]
	308996.439	(0.030)	36(3,34)	-	35(3,33)				[83039]
	311205.304	(0.030)	36(13,24)	-	35(13,23)				[83039]
	311268.036	(0.030)	36(9,28)	-	35(9,27)				[83039]
	311306.870	(0.030)	36(15,22)	-	35(15,21)				[83039]
	311459.616	(0.030)	36(17,20)	-	35(17,19)				[83039]
	311611.879	(0.030)	36(7,30)	-	35(7,29)				[83039]
	311615.304	(0.030)	36(7,29)	-	35(7,28)				[83039]
	311652.431	(0.030)	36(19,18)	-	35(19,17)				[83039]
	311769.796	(0.030)	37(2,36)	-	36(2,35)				[83039]
	311879.554	(0.030)	36(21,16)	-	35(21,15)				[83039]
	311910.203	(0.030)	36(4,33)	-	35(4,32)				[83039]
	311971.139	(0.030)	36(6,31)	-	35(6,30)				[83039]
	312035.945	(0.030)	36(6,30)	-	35(6,29)				[83039]
	312137.370	(0.030)	36(23,14)	-	35(23,13)				[83039]
	312167.085	(0.030)	37(1,36)	-	36(1,35)				[83039]
	312226.217	(0.030)	36(2,34)	-	35(2,33)				[83039]
	312372.976	(0.030)	36(5,32)	-	35(5,31)				[83039]
	312423.035	(0.030)	36(25,12)	-	35(25,11)				[83039]
	312735.206	(0.030)	36(27,10)	-	35(27,9)				[83039]
	313072.181	(0.030)	36(29,8)	-	35(29,7)				[83039]
	313142.560	(0.030)	36(5,31)	-	35(5,30)				[83039]
	313433.174	(0.030)	36(31,6)	-	35(31,5)				[83039]
	313520.719	(0.030)	38(1,38)	-	37(1,37)				[83039]
	313532.888	(0.030)	38(0,38)	-	37(0,37)				[83039]
	313622.520	(0.030)	36(32,5)	-	35(32,4)				[83039]
	313817.501	(0.030)	36(33,4)	-	35(33,3)				[83039]
	316266.804	(0.030)	36(4,32)	-	35(4,31)				[83039]
	317318.688	(0.030)	37(3,35)	-	36(3,34)				[83039]
	317687.681	(0.030)	36(3,33)	-	35(3,32)				[83039]

Table 21.1. Molecular constants for
1,2-butadiene (methyl allene).

Parameter	Value
<u>Rotational Constants</u> [present]	
A (MHz)	34023.(46)
B (MHz)	4201.278(14)
C (MHz)	3928.099(15)
Δ_J (kHz)	1.78(16)
Δ_{JK} (kHz)	-56.82(63)
δ_J (kHz)	0.32(25)
<u>Internal Rotation Constants</u> ^a [present]	
I_α (u Å ²)	3.103
θ	38.16°
V_3 (cm ⁻¹)	556.94(87)
Δ_0 (MHz)	-151.9
β (rad)	0.09673
ρ	0.16503
<u>Dipole Moment</u> [57016]	
μ_a (D)	0.394(2)
μ_b (D)	0.070(1)

^aOnly the rotational constants and V_3 were fit.

TABLE 21.2. Microwave spectrum of methylallene

C₃H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	v_1	Sym.	Ref.
H ₂ CCCHCH ₃	15985.82	(0.03)	2(1, 2) - 1(1, 1)	0	A	[57016]
	15987.84	(0.03)	2(1, 2) - 1(1, 1)	0	E	[57016]
	16256.76	(0.03)	2(0, 2) - 1(0, 1)	0	E	[57016]
	16256.93	(0.03)	2(0, 2) - 1(0, 1)	0	A	[57016]
	16529.90	(0.03)	2(1, 1) - 1(1, 0)	0	E	[57016]
	16532.29	(0.03)	2(1, 1) - 1(1, 0)	0	A	[57016]
	23977.46	(0.03)	3(1, 3) - 2(1, 2)	0	A	[57016]
	23977.89	(0.03)	3(1, 3) - 2(1, 2)	0	E	[57016]
	24380.36	(0.03)	3(0, 3) - 2(0, 2)	0	E	[57016]
	24380.63	(0.03)	3(0, 3) - 2(0, 2)	0	A	[57016]
	24389.35	(0.03)	3(2, 2) - 2(2, 1)	0	A	[57016]
	24392.80	(0.03)	3(2, 2) - 2(2, 1)	0	E	[57016]
	24393.20	(0.03)	3(2, 1) - 2(2, 0)	0	E	[57016]
	24396.90	(0.03)	3(2, 1) - 2(2, 0)	0	A	[57016]
	24796.20	(0.03)	3(1, 2) - 2(1, 1)	0	E	[57016]
	24797.09	(0.03)	3(1, 2) - 2(1, 1)	0	A	[57016]
	31967.61	(0.03)	4(1, 4) - 3(1, 3)	0	A	[57016]
	31967.67	(0.03)	4(1, 4) - 3(1, 3)	0	E	[57016]
	32498.28	(0.03)	4(0, 4) - 3(0, 3)	0	E	[57016]
	32498.63	(0.03)	4(0, 4) - 3(0, 3)	0	A	[57016]
	32517.58	(0.03)	4(2, 3) - 3(2, 2)	0	A	[57016]
	32525.00	(0.03)	4(2, 3) - 3(2, 2)	0	E	[57016]
	32525.00	(0.03)	4(3, 2) - 3(3, 1)	0	A,E	[57016]
	32525.00	(0.03)	4(3, 1) - 3(3, 0)	0	A,E	[57016]
	32528.10	(0.03)	4(2, 2) - 3(2, 1)	0	E	[57016]
	32536.26	(0.03)	4(2, 2) - 3(2, 1)	0	A	[57016]
	33059.64	(0.03)	4(1, 3) - 3(1, 2)	0	E	[57016]
	33060.34	(0.03)	4(1, 3) - 3(1, 2)	0	A	[57016]

Table 22.1. Molecular constants for bicyclo[1.1.0.]butane.

Species	A (MHz)	B (MHz)	C (MHz)	Reference
<u>Rotational Constants</u>				
$\text{CH}_2\text{CHCHCH}_2$	17311.974(40)	9313.516(32)	8393.521(30)	[present]
$\text{CH}_2\text{}^{13}\text{CHCHCH}_2$ (1- ^{13}C)	16934.17(14)	9298.37(18)	8316.53(14)	[69057]
$^{13}\text{CH}_2\text{CHCHCH}_2$ (2- ^{13}C)	17256.84(13)	9085.62(17)	8220.44(13)	[69057]
$\text{CD}_2\text{CHCHCH}_2$ (7,9- D_2)	16221.47(13)	8164.35(17)	7670.79(13)	[69057]
$\text{CH}_2\text{CDCHCH}_2$ (5-D)	15554.92(8)	9151.50(10)	8077.18(8)	[69057]
<u>Dipole Moment</u> [66041]				
μ_c	0.67 _s (1 _o) D			
<u>Zeeman Constants</u> [72061]				
g_{aa}	0.0593(2) ^a μ_N			
g_{bb}	0.0025(2) ^a μ_N			
g_{cc}	0.0412(2) ^a μ_N			
$2\chi_{aa}-\chi_{bb}-\chi_{cc}$	$-5.9(3)\times 10^{-6}\text{erg/G}^2\cdot\text{mol}$			
$-\chi_{aa}+2\chi_{bb}-\chi_{cc}$	$21.1(3)\times 10^{-6}\text{erg/G}^2\cdot\text{mol}$			

^aSign not determined, but positive values are favored.

TABLE 22.2. Microwave spectrum of bicyclo[1.1.0]butane

C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
CHCH ₂ CHCH ₂	20927.71	(0.02)	4(2, 3) - 4(1, 3)	[66041]
	22664.24	(0.02)	3(2, 2) - 3(1, 2)	[72061]
	23995.40	(0.02)	2(2, 1) - 2(1, 1)	[72061]
	26420.70	(0.02)	2(0, 2) - 1(1, 0)	[72061]
	26625.57	(0.02)	1(1, 0) - 0(0, 0)	[72061]
¹³ CHCH ₂ CHCH ₂	26830.19	(0.02)	2(2, 0) - 2(1, 2)	[72061]
	17444.92	(0.10)	5(2, 4) - 5(1, 4)	[69057]
	19653.46	(0.10)	4(2, 3) - 4(1, 3)	[69057]
	21492.81	(0.10)	3(2, 2) - 3(1, 2)	[69057]
	22907.47	(0.10)	2(2, 1) - 2(1, 1)	[69057]
CH ¹³ CH ₂ CHCH ₂	26232.58	(0.10)	1(1, 0) - 0(0, 0)	[69057]
	26523.32	(0.10)	2(0, 2) - 1(1, 0)	[69057]
	19627.78	(0.10)	5(2, 4) - 5(1, 4)	[69057]
	21617.08	(0.10)	4(2, 3) - 4(1, 3)	[69057]
	23258.20	(0.10)	3(2, 2) - 3(1, 2)	[69057]
CDCH ₂ CHCH ₂	24513.66	(0.10)	2(2, 1) - 2(1, 1)	[69057]
	25510.43	(0.10)	2(0, 2) - 1(1, 0)	[69057]
	26342.53	(0.10)	1(1, 0) - 0(0, 0)	[69057]
	19210.19	(0.10)	2(2, 1) - 2(1, 1)	[69057]
	22557.42	(0.10)	2(2, 0) - 2(1, 2)	[69057]
CHCD ₂ CHCH ₂	24706.50	(0.10)	1(1, 0) - 0(0, 0)	[69057]
	24728.46	(0.10)	3(2, 1) - 3(1, 3)	[69057]
	26855.28	(0.10)	2(0, 2) - 1(1, 0)	[69057]
	28156.41	(0.10)	4(2, 2) - 4(1, 4)	[69057]
	21306.68	(0.10)	5(2, 4) - 5(1, 4)	[69057]
	22486.78	(0.10)	4(2, 3) - 4(1, 3)	[69057]
	23097.49	(0.10)	2(0, 2) - 1(1, 0)	[69057]
23445.13	(0.10)	3(2, 2) - 3(1, 2)	[69057]	
24171.30	(0.10)	2(2, 1) - 2(1, 1)	[69057]	
24385.89	(0.10)	1(1, 0) - 0(0, 0)	[69057]	

Table 23.1. Molecular constants for cyclobutene and its ^{13}C isotopic species.

Parameter	Cyclobutene	1- ^{13}C -Cyclobutene	3- ^{13}C -Cyclobutene
<u>Rotational Constants</u>			
A'' (MHz)	12892.8825(23)	12784.7842(71)	12742.881(16)
B'' (MHz)	12226.1058(22)	12015.5953(71)	12033.857(16)
C'' (MHz)	6816.2674(13)	6720.5173(65)	6714.547(14)
τ_1 (MHz)	-0.047866(2693)	-0.05134(301)	-0.04776(664)
τ_2 (MHz)	-0.012535(902)	-0.01398(101)	-0.01285(223)
τ_3^a (MHz)	1.80(3)	1.52(3)	1.58(8)
τ_{aaaa} (MHz)	-0.028287(839)	-0.030417(940)	-0.03002(208)
τ_{bbbb} (MHz)	-0.026388(860)	-0.028334(961)	-0.02762(212)
<u>Electric Dipole Moment</u> [65029]			
μ	0.131(1) D		
<u>Zeeman Constants</u> [70063]			
g_{aa}	-0.0516(7) μ_N		
g_{bb}	-0.0663(7) μ_N		
g_{cc}	-0.0219(6) μ_N		
$2\chi_{aa}-\chi_{bb}-\chi_{cc}$	$-0.9(5)\times 10^{-6}\text{erg/G}^2\cdot\text{mol}$		
$-\chi_{aa}+2\chi_{bb}-\chi_{cc}$	$5.0(7)\times 10^{-6}\text{erg/G}^2\cdot\text{mol}$		
Q_{aa}	$-0.3(6)\times 10^{-26}\text{esu}\cdot\text{cm}^2$		
Q_{bb}	$1.6(7)\times 10^{-26}\text{esu}\cdot\text{cm}^2$		
Q_{cc}	$-1.3(10)\times 10^{-26}\text{esu}\cdot\text{cm}^2$		

^aThe value of τ_3 is fixed by setting $R_6 = 0$.

Table 23.2. Molecular constants for monodeutero-species of cyclobutene.

Parameter	DC=CHCH ₂ CH ₂	HC=CHCHDCH ₂
<u>Rotational Constants</u>		
A'' (MHz)	12658.7572(50)	12419.2632(50)
B'' (MHz)	11220.9574(54)	11431.6151(51)
C'' (MHz)	6432.0155(37)	6557.7960(33)
τ_1 (MHz)	-0.03095(416)	-0.04505(386)
τ_2 (MHz)	-0.00833(138)	-0.01290(129)
τ_3^a (MHz)	0.62(2)	0.92(3)
τ_{aaaa} (MHz)	-0.0297(11)	-0.0316(11)
τ_{bbbb} (MHz)	-0.0217(13)	-0.0268(12)

^aThe value of τ_3 is fixed by setting $R_6 = 0$.

TABLE 23.3. Microwave spectrum of cyclobutene

C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.	
CHCHCH ₂ CH ₂	8978.350	(0.050)	7(6, 1) - 7(6, 2)	[65029]	
	10799.790	(0.050)	6(5, 1) - 6(5, 2)	[65029]	
HC=CH H ₂ C-CH ₂	12117.960	(0.050)	12(10, 2) - 12(10, 3)	[65029]	
	12505.920	(0.050)	5(4, 1) - 5(4, 2)	[65029]	
HC=CH H ₂ C-CH ₂	12692.450	(0.050)	23(19, 4) - 23(19, 5)	[69056]	
	13689.510	(0.050)	28(23, 5) - 28(23, 6)	[69056]	
	14013.860	(0.050)	4(3, 1) - 4(3, 2)	[65029]	
	14538.640	(0.050)	17(14, 3) - 17(14, 4)	[69056]	
	14844.600	(0.050)	11(9, 2) - 11(9, 3)	[65029]	
	15266.996	(0.010)	3(2, 1) - 3(2, 2)	[70063]	
	16229.412	(0.010)	2(1, 1) - 2(1, 2)	[70063]	
	16396.190	(0.050)	22(18, 4) - 22(18, 5)	[69056]	
	17566.250	(0.050)	10(8, 2) - 10(8, 3)	[69056]	
	17791.170	(0.050)	27(22, 5) - 27(22, 6)	[69056]	
	18006.690	(0.050)	16(13, 3) - 16(13, 4)	[69056]	
	18287.640	(0.050)	2(2, 1) - 2(0, 2)	[65029]	
	19042.345	(0.005)	1(0, 1) - 0(0, 0)	[70063]	
	19551.500	(0.020)	3(3, 1) - 3(1, 2)	[65029]	
	20157.350	(0.050)	9(7, 2) - 9(7, 3)	[69056]	
	20483.820	(0.050)	21(17, 4) - 21(17, 5)	[69056]	
	21580.450	(0.050)	15(12, 3) - 15(12, 4)	[69056]	
	22508.530	(0.050)	8(6, 2) - 8(6, 3)	[69056]	
	24305.940	(0.050)	5(5, 1) - 5(3, 2)	[69056]	
	24526.770	(0.050)	7(5, 2) - 7(5, 3)	[69056]	
	24791.660	(0.050)	20(16, 4) - 20(16, 5)	[69056]	
	25105.050	(0.050)	14(11, 3) - 14(11, 4)	[69056]	
	26140.110	(0.050)	6(4, 2) - 6(4, 3)	[69056]	
	27312.200	(0.050)	5(3, 2) - 5(3, 3)	[69056]	
	27339.550	(0.050)	25(20, 5) - 25(20, 6)	[69056]	
	28061.070	(0.050)	4(2, 2) - 4(2, 3)	[69056]	
	28097.620	(0.050)	6(6, 1) - 6(4, 2)	[69056]	
	28435.670	(0.050)	13(10, 3) - 13(10, 4)	[69056]	
	28753.690	(0.050)	3(2, 2) - 3(0, 3)	[69056]	
	28924.070	(0.050)	4(3, 2) - 4(1, 3)	[69056]	
	29143.220	(0.050)	19(15, 4) - 19(15, 5)	[69056]	
	29285.270	(0.050)	5(4, 2) - 5(2, 3)	[69056]	
	29320.590	(0.050)	30(24, 6) - 30(24, 7)	[69056]	
	29951.850	(0.050)	6(5, 2) - 6(3, 3)	[69056]	
	31072.440	(0.050)	7(6, 2) - 7(4, 3)	[69056]	
	31442.020	(0.050)	12(9, 3) - 12(9, 4)	[69056]	
	32428.970	(0.050)	24(19, 5) - 24(19, 6)	[69056]	
	32674.801	(0.010)	2(1, 2) - 1(1, 1)	[70063]	
	32825.200	(0.050)	8(7, 2) - 8(5, 3)	[69056]	
	32934.350	(0.050)	7(7, 1) - 7(5, 2)	[69056]	
	33283.680	(0.050)	2(0, 2) - 1(0, 1)	[65029]	
	33365.070	(0.050)	18(14, 4) - 18(14, 5)	[69056]	
	34015.330	(0.050)	11(8, 3) - 11(8, 4)	[69056]	
	35067.080	(0.050)	29(23, 6) - 29(23, 7)	[69056]	
	¹³ CHCHCH ₂ CH ₂	13173.610	(0.050)	26(21, 5) - 26(21, 6)	[69056]
		13377.110	(0.050)	16(13, 3) - 16(13, 4)	[69056]
14782.630		(0.050)	3(2, 1) - 3(2, 2)	[69056]	
15141.950		(0.050)	10(8, 2) - 10(8, 3)	[69056]	
15885.150		(0.050)	2(1, 1) - 2(1, 2)	[69056]	
16695.060		(0.050)	30(24, 6) - 30(24, 7)	[69056]	
17712.640		(0.050)	20(16, 4) - 20(16, 5)	[69056]	
18027.730		(0.050)	9(7, 2) - 9(7, 3)	[69056]	
18270.580		(0.050)	2(2, 1) - 2(0, 2)	[65956]	
18736.100		(0.050)	1(0, 1) - 0(0, 0)	[69056]	
19776.840		(0.050)	3(3, 1) - 3(1, 2)	[69056]	
20729.610		(0.050)	8(6, 2) - 8(6, 3)	[69056]	
20827.780		(0.050)	14(11, 3) - 14(11, 4)	[69056]	
21841.250		(0.050)	29(23, 6) - 29(23, 7)	[69056]	
22130.720		(0.050)	4(4, 1) - 4(2, 2)	[69056]	
22448.790		(0.050)	24(19, 5) - 24(19, 6)	[69056]	
23117.750		(0.050)	7(5, 2) - 7(5, 3)	[69056]	
25084.910		(0.050)	6(4, 2) - 6(4, 3)	[69056]	
25534.090		(0.050)	5(5, 1) - 5(3, 2)	[69056]	

TABLE 23.3. Microwave spectrum of cyclobutene — Continued

C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
	26558.880	(0.050)	5(3, 2) - 5(3, 3)	[69056]
	26563.530	(0.050)	33(26, 7) - 33(26, 8)	[69056]
	26842.920	(0.050)	18(14, 4) - 18(14, 5)	[69056]
	27527.900	(0.050)	4(2, 2) - 4(2, 3)	[69056]
	27581.840	(0.050)	28(22, 6) - 28(22, 7)	[69056]
	28163.070	(0.050)	12(9, 3) - 12(9, 4)	[69056]
	28449.390	(0.050)	3(2, 2) - 3(0, 3)	[69056]
	28681.020	(0.050)	4(3, 2) - 4(1, 3)	[69056]
	29174.680	(0.050)	5(4, 2) - 5(2, 3)	[69056]
	30089.690	(0.050)	6(5, 2) - 6(3, 3)	[69056]
	30116.980	(0.050)	6(6, 1) - 6(4, 2)	[69056]
	30890.660	(0.050)	12(9, 3) - 12(8, 4)	[69056]
	31630.060	(0.050)	7(6, 2) - 7(4, 3)	[69056]
	31902.800	(0.050)	17(14, 3) - 17(13, 4)	[69056]
	32177.040	(0.050)	2(1, 2) - 1(1, 1)	[69056]
	32804.780	(0.050)	11(8, 3) - 11(7, 4)	[69056]
	32868.360	(0.050)	2(0, 2) - 1(0, 1)	[69056]
	33105.740	(0.050)	32(25, 7) - 32(25, 8)	[69056]
	33191.120	(0.050)	22(17, 5) - 22(17, 6)	[69056]
	33678.740	(0.050)	27(21, 6) - 27(21, 7)	[69056]
	34030.040	(0.050)	8(7, 2) - 8(5, 3)	[69056]
	34347.640	(0.050)	15(13, 2) - 15(12, 3)	[69056]
	34737.930	(0.050)	10(7, 3) - 10(6, 4)	[69056]
	34878.280	(0.050)	19(15, 4) - 19(14, 5)	[69056]
	35432.940	(0.050)	18(15, 3) - 18(14, 4)	[69056]
	35551.980	(0.050)	20(16, 4) - 20(15, 5)	[69056]
	35908.370	(0.050)	7(7, 1) - 7(5, 2)	[69056]
	13108.050	(0.050)	22(18, 4) - 22(18, 5)	[69056]
	13436.270	(0.050)	27(22, 5) - 27(22, 6)	[69056]
	14937.670	(0.050)	3(2, 1) - 3(2, 2)	[69056]
	15670.680	(0.050)	16(13, 3) - 16(13, 4)	[69056]
	15957.860	(0.050)	2(1, 1) - 2(1, 2)	[69056]
	16317.070	(0.050)	10(8, 2) - 10(8, 3)	[69056]
	17638.860	(0.050)	26(21, 5) - 26(21, 6)	[69056]
	18151.190	(0.050)	2(2, 1) - 2(0, 2)	[69056]
	18748.400	(0.050)	1(0, 1) - 0(0, 0)	[69056]
	19035.370	(0.050)	9(7, 2) - 9(7, 3)	[69056]
	19515.360	(0.050)	3(3, 1) - 3(1, 2)	[69056]
	21242.280	(0.050)	20(16, 4) - 20(16, 5)	[69056]
	21537.330	(0.050)	8(6, 2) - 8(6, 3)	[69056]
	21633.300	(0.050)	4(4, 1) - 4(2, 2)	[69056]
	22834.550	(0.050)	30(24, 6) - 30(24, 7)	[69056]
	22946.770	(0.050)	14(11, 3) - 14(11, 4)	[69056]
	23714.640	(0.050)	7(5, 2) - 7(5, 3)	[69056]
	24689.020	(0.050)	5(5, 1) - 5(3, 2)	[69056]
	25479.970	(0.050)	6(4, 2) - 6(4, 3)	[69056]
	26781.140	(0.050)	5(3, 2) - 5(3, 3)	[69056]
	27458.760	(0.050)	24(19, 5) - 24(19, 6)	[69056]
	27623.440	(0.050)	4(2, 2) - 4(2, 3)	[69056]
	28412.270	(0.050)	3(2, 2) - 3(0, 3)	[69056]
	28418.280	(0.050)	29(23, 6) - 29(23, 7)	[69056]
	28608.300	(0.050)	4(3, 2) - 4(1, 3)	[69056]
	28813.330	(0.050)	6(6, 1) - 6(4, 2)	[69056]
	29024.700	(0.050)	5(4, 2) - 5(2, 3)	[69056]
	29735.270	(0.050)	12(9, 3) - 12(9, 4)	[69056]
	29794.850	(0.050)	6(5, 2) - 6(3, 3)	[69056]
	30124.010	(0.050)	18(14, 4) - 18(14, 5)	[69056]
	30185.340	(0.050)	17(14, 3) - 17(13, 4)	[69056]
	31090.770	(0.050)	7(6, 2) - 7(4, 3)	[69056]
	31462.860	(0.050)	15(13, 2) - 15(12, 3)	[69056]
	31779.600	(0.050)	12(9, 3) - 12(8, 4)	[69056]
	32177.360	(0.050)	2(1, 2) - 1(1, 1)	[69056]
	32775.260	(0.050)	18(15, 3) - 18(14, 4)	[69056]
	32820.190	(0.050)	2(0, 2) - 1(0, 1)	[69056]
	33115.040	(0.050)	8(7, 2) - 8(5, 3)	[69056]
	33659.350	(0.050)	11(8, 3) - 11(7, 4)	[69056]
	34052.600	(0.050)	7(7, 1) - 7(5, 2)	[69056]

CHCH¹³CH₂CH₂

TABLE 23.3. Microwave spectrum of cyclobutene — Continued

C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.	
CDCHCH ₂ CH ₂	34296.890	(0.050)	28(22, 6) - 28(22, 7)	[69056]	
	34912.930	(0.050)	20(16, 4) - 20(15, 5)	[69056]	
	34964.950	(0.050)	10(9, 2) - 10(8, 3)	[69056]	
	35101.650	(0.050)	33(26, 7) - 33(26, 8)	[69056]	
	35163.070	(0.050)	19(15, 4) - 19(14, 5)	[69056]	
	35438.630	(0.050)	10(7, 3) - 10(6, 4)	[69056]	
	12403.970	(0.050)	3(2, 1) - 3(2, 2)	[69056]	
	13781.880	(0.050)	22(16, 6) - 22(16, 7)	[69056]	
	14366.730	(0.050)	2(1, 1) - 2(1, 2)	[69056]	
	15068.330	(0.050)	7(5, 2) - 7(5, 3)	[69056]	
	16523.210	(0.050)	25(18, 7) - 25(18, 8)	[69056]	
	16866.450	(0.050)	18(13, 5) - 18(13, 6)	[69056]	
	17652.930	(0.050)	1(0, 1) - 0(0, 0)	[69056]	
	18680.110	(0.050)	2(2, 1) - 2(1, 2)	[69056]	
	18862.600	(0.050)	6(4, 2) - 6(4, 3)	[69056]	
	18958.120	(0.050)	2(2, 1) - 2(0, 2)	[69056]	
	19090.760	(0.050)	1(1, 1) - 0(0, 0)	[69056]	
	19264.820	(0.050)	14(10, 4) - 14(10, 5)	[69056]	
	19452.160	(0.050)	28(20, 8) - 28(20, 9)	[69056]	
	20203.160	(0.050)	10(7, 3) - 10(7, 4)	[69056]	
	22183.560	(0.050)	5(3, 2) - 5(3, 3)	[69056]	
	22323.780	(0.050)	3(3, 1) - 3(1, 2)	[69056]	
	24027.880	(0.050)	24(17, 7) - 24(17, 8)	[69056]	
	24742.360	(0.050)	4(2, 2) - 4(2, 3)	[69056]	
	25204.180	(0.050)	9(6, 3) - 9(6, 4)	[69056]	
	27733.050	(0.050)	3(2, 2) - 3(0, 3)	[69056]	
	27763.050	(0.050)	4(4, 1) - 4(2, 2)	[69056]	
	27897.880	(0.050)	27(19, 8) - 27(19, 9)	[69056]	
	28057.100	(0.050)	20(14, 6) - 20(14, 7)	[69056]	
	28619.590	(0.050)	4(3, 2) - 4(1, 3)	[69056]	
	29684.540	(0.050)	8(5, 3) - 8(5, 4)	[69056]	
	30238.940	(0.050)	2(0, 2) - 1(1, 1)	[69056]	
	30516.930	(0.050)	2(1, 2) - 1(1, 1)	[69056]	
	30797.620	(0.050)	16(11, 5) - 16(11, 6)	[69056]	
	31541.360	(0.050)	12(8, 4) - 12(8, 5)	[69056]	
	31676.740	(0.050)	2(0, 2) - 1(0, 1)	[69056]	
	31954.750	(0.050)	2(1, 2) - 1(0, 1)	[69056]	
	31957.870	(0.050)	30(21, 9) - 30(21,10)	[69056]	
	31957.870	(0.050)	30(21, 9) - 30(21,10)	[69056]	
	35483.300	(0.050)	5(5, 1) - 5(3, 2)	[69056]	
	CHCHCH ₂ CHD	12803.540	(0.050)	18(14, 4) - 18(14, 5)	[69056]
		13230.540	(0.050)	3(2, 1) - 3(2, 2)	[69056]
		13230.540	(0.050)	3(2, 1) - 3(2, 2)	[69056]
		13762.560	(0.050)	22(17, 5) - 22(17, 6)	[69056]
		14399.510	(0.050)	26(20, 6) - 26(20, 7)	[69056]
14620.860		(0.050)	2(1, 1) - 2(1, 2)	[69056]	
14764.690		(0.050)	30(23, 7) - 30(23, 8)	[69056]	
15995.340		(0.050)	8(6, 2) - 8(6, 3)	[69056]	
17583.810		(0.050)	2(2, 1) - 2(1, 2)	[69056]	
17719.250		(0.050)	2(2, 1) - 2(0, 2)	[69056]	
17989.550		(0.050)	1(0, 1) - 0(0, 0)	[69056]	
18977.240		(0.050)	1(1, 1) - 0(0, 0)	[69056]	
19040.630		(0.050)	7(5, 2) - 7(5, 3)	[69056]	
19553.270		(0.050)	12(9, 3) - 12(9, 4)	[69056]	
19805.750		(0.050)	3(3, 1) - 3(1, 2)	[69056]	
21718.690		(0.050)	6(4, 2) - 6(4, 3)	[69056]	
22354.920		(0.050)	16(12, 4) - 16(12, 5)	[69056]	
23137.830		(0.050)	4(4, 1) - 4(2, 2)	[69056]	
23865.560		(0.050)	5(3, 2) - 5(3, 3)	[69056]	
24527.850		(0.050)	20(15, 5) - 20(15, 6)	[69056]	
25376.300		(0.050)	4(2, 2) - 4(2, 3)	[69056]	
26159.620		(0.050)	24(18, 6) - 24(18, 7)	[69056]	
26928.310		(0.050)	3(2, 2) - 3(0, 3)	[69056]	
27317.500		(0.050)	28(21, 7) - 28(21, 8)	[69056]	
27342.630		(0.050)	4(3, 2) - 4(1, 3)	[69056]	
27529.140		(0.050)	10(7, 3) - 10(7, 4)	[69056]	
27955.630		(0.050)	5(5, 1) - 5(3, 2)	[69056]	

TABLE 23.3. Microwave spectrum of cyclobutene — Continued

C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
	30830.500	(0.050)	9(6, 3) - 9(6, 4)	[69056]
	30969.960	(0.050)	2(0, 2) - 1(1, 1)	[69056]
	31105.370	(0.050)	2(1, 2) - 1(1, 1)	[69056]
	31957.590	(0.050)	2(0, 2) - 1(0, 1)	[69056]
	32093.040	(0.050)	2(1, 2) - 1(0, 1)	[69056]
	32357.000	(0.050)	14(10, 4) - 14(10, 5)	[69056]

Table 24.1. Molecular constants for 1-methylcyclopropene.

Parameter	CH ₃ CCH ₂ CH	
	Ground State	Torsional State
<u>Rotational Constants</u>		
A (MHz)	20549.975(92)	20322.347
B (MHz)	6357.084(28)	6342.620
C (MHz)	5176.431(17)	5172.440
Δ_J (kHz)	2.67(134)	
Δ_{JK} (kHz)	9.98(314)	
Δ_K (kHz)	77.0(72)	
δ_J (kHz)	0.39(6)	
δ_K (kHz)	6.9(50)	
Reference	[present]	[69066]
<u>Internal Rotation Constants</u>		
I_α (u Å ²)	3.124 ^a	3.124 ^a
θ	6.16 ^a	
λ_a	0.99423	0.9922(65)
λ_b	-0.10730	-0.1262(52)
ν_3 (cm ⁻¹)	488.27(28)	483.3(7)
Reference	[present]	[69066]
<u>Dipole Moment [69066]</u>		
μ_a (D)	0.818(8)	
μ_b (D)	0.19(2)	

^aAssumed parameter.

Comments: In reference [67066] a quantum number error $6_{16}-6_{16}$ has been corrected to $6_{16}-6_{15}$ and the $8_{27}-8_{26}$ transition deviates by 1 MHz and thus, was not fit.

TABLE 24.2. Microwave spectrum of methyl cyclopropene

C₄H₆


Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$	$- J''(K_{-1}, K_{+1})$	ν_1	Sym.	Ref.
CH ₃ CCHCH ₂ 	9311.70	(0.20)	6(1, 6)	- 5(2, 3)	0	A	[69066]
	10715.37	(0.20)	12(3, 9)	- 12(3, 10)	0	A	[69066]
	10727.09	(0.20)	12(3, 9)	- 12(3, 10)	0	E	[69066]
	11515.16	(0.20)	1(0, 1)	- 0(0, 0)	1	A,E	[69066]
	11533.51	(0.20)	1(0, 1)	- 0(0, 0)	0	A,E	[69066]
	11787.58	(0.20)	4(1, 3)	- 4(1, 4)	0	A	[69066]
	11787.68	(0.20)	4(1, 3)	- 4(1, 4)	0	E	[69066]
	12435.58	(0.20)	17(4, 13)	- 17(4, 14)	0	A	[69066]
	12453.93	(0.20)	8(2, 6)	- 8(2, 7)	0	A	[69066]
	12461.36	(0.20)	8(2, 6)	- 8(2, 7)	0	E	[69066]
	15371.51	(0.20)	1(1, 0)	- 1(0, 1)	0	E	[69066]
	15379.86	(0.20)	1(1, 0)	- 1(0, 1)	0	A	[69066]
	16621.89	(0.20)	2(1, 1)	- 2(0, 2)	0	E	[69066]
	16630.94	(0.20)	2(1, 1)	- 2(0, 2)	0	A	[69066]
	17635.13	(0.20)	5(1, 4)	- 5(1, 5)	0	A	[69066]
	18380.64	(0.20)	3(1, 2)	- 3(0, 3)	1	A	[69066]
	18627.85	(0.20)	3(1, 2)	- 3(0, 3)	0	E	[69066]
	18636.95	(0.20)	3(1, 2)	- 3(0, 3)	0	A	[69066]
	19024.97	(0.20)	3(1, 2)	- 3(0, 3)	1	E	[69066]
	21230.55	(0.20)	3(0, 3)	- 2(1, 2)	0	A	[69066]
	21240.35	(0.20)	3(0, 3)	- 2(1, 2)	0	E	[69066]
	21384.95	(0.20)	3(0, 3)	- 2(1, 2)	1	A	[69066]
	21531.01	(0.20)	4(1, 3)	- 4(0, 4)	0	E	[69066]
	21539.86	(0.20)	4(1, 3)	- 4(0, 4)	0	A	[69066]
	21577.29	(0.20)	3(0, 3)	- 2(1, 2)	1	E	[69066]
	21859.99	(0.20)	2(1, 2)	- 1(1, 1)	1	A	[69066]
	21886.30	(0.20)	2(1, 2)	- 1(1, 1)	0	A	[69066]
	21887.22	(0.20)	2(1, 2)	- 1(1, 1)	0	E	[69066]
	22322.66	(0.20)	2(1, 2)	- 1(1, 1)	1	E	[69066]
	22959.79	(0.20)	2(0, 2)	- 1(0, 1)	1	A	[69066]
	22961.32	(0.20)	2(0, 2)	- 1(0, 1)	1	E	[69066]
	22996.37	(0.20)	2(0, 2)	- 1(0, 1)	0	A,E	[69066]
	23729.21	(0.20)	2(1, 1)	- 1(1, 0)	1	E	[69066]
	24200.36	(0.20)	2(1, 1)	- 1(1, 0)	1	A	[69066]
	24246.60	(0.20)	2(1, 1)	- 1(1, 0)	0	E	[69066]
	24247.53	(0.20)	2(1, 1)	- 1(1, 0)	0	A	[69066]
	24572.15	(0.20)	6(1, 5)	- 6(1, 6)	0	E	[69066]
	24572.59	(0.20)	6(1, 5)	- 6(1, 6)	0	A	[69066]
	24828.50	(0.20)	1(1, 1)	- 0(0, 0)	1	E	[69066]
	25494.80	(0.20)	1(1, 1)	- 0(0, 0)	1	A	[69066]
	25721.74	(0.20)	1(1, 1)	- 0(0, 0)	0	E	[69066]
	25732.61	(0.20)	1(1, 1)	- 0(0, 0)	0	A	[69066]
	30621.58	(0.20)	6(1, 5)	- 6(0, 6)	0	E	[69066]
	30629.55	(0.20)	6(1, 5)	- 6(0, 6)	0	A	[69066]
	32747.21	(0.20)	3(1, 3)	- 2(1, 2)	1	A	[69066]
	32786.00	(0.20)	3(1, 3)	- 2(1, 2)	0	A	[69066]
	32786.23	(0.20)	3(1, 3)	- 2(1, 2)	0	E	[69066]
	32986.28	(0.20)	3(1, 3)	- 2(1, 2)	1	E	[69066]
	33398.01	(0.20)	11(2, 9)	- 11(2, 10)	0	A	[69066]
	33407.93	(0.20)	11(2, 9)	- 11(2, 10)	0	E	[69066]
	34265.23	(0.20)	3(0, 3)	- 2(0, 2)	1	A	[69066]
	34272.90	(0.20)	3(0, 3)	- 2(0, 2)	1	E	[69066]
	34319.62	(0.20)	3(0, 3)	- 2(0, 2)	0	E	[69066]
	34319.78	(0.20)	3(0, 3)	- 2(0, 2)	0	A	[69066]
	34544.95	(0.20)	3(2, 2)	- 2(2, 1)	1	A	[69066]
	34599.99	(0.20)	3(2, 2)	- 2(2, 1)	0	A	[69066]
	34633.68	(0.20)	3(2, 2)	- 2(2, 1)	0	E	[69066]
34680.80	(0.20)	3(2, 1)	- 2(2, 0)	1	E	[69066]	
34684.4	(0.2)	3(2, 2)	- 2(2, 1)	1	E	[69066]	
34824.96	(0.20)	3(2, 1)	- 2(2, 0)	1	A	[69066]	
34847.38	(0.20)	3(2, 1)	- 2(2, 0)	0	E	[69066]	
34880.95	(0.20)	3(2, 1)	- 2(2, 0)	0	A	[69066]	
35839.23	(0.20)	2(0, 2)	- 1(0, 1)	1	A	[69066]	
36018.19	(0.20)	3(1, 2)	- 2(1, 1)	1	A	[69066]	
36075.46	(0.20)	2(1, 2)	- 1(0, 1)	0	E	[69066]	
36085.55	(0.20)	2(1, 2)	- 1(0, 1)	0	A	[69066]	
36255.04	(0.20)	3(1, 2)	- 2(1, 1)	1	A	[69066]	

TABLE 24.2. Microwave spectrum of methyl cyclopropene — Continued

C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_1	Sym.	Ref.
	36325.16	(0.20)	3(1, 2) - 2(1, 1)	0	E	[69066]
	36325.49	(0.20)	3(1, 2) - 2(1, 1)	0	A	[69066]

Table 25.1. Molecular constants for methylene cyclopropane.

Parameter	Value
A'' (MHz)	19415.25(88)
B'' (MHz)	6877.1615(65)
C'' (MHz)	5445.1776(80)
τ_1 (MHz)	-0.09252(813)
τ_2 (MHz)	-0.01784(239)
τ_3^a (MHz)	0.53(22)
τ_{bbbb} (MHz)	-0.0099(20)
τ_{cccc} (MHz)	-0.0052(24)

Dipole Moment [70062] μ_a (D) 0.402Zeeman Constants [70063]

g_{aa} (μ_N)	-0.0672(7)
g_{bb} (μ_N)	-0.0231(4)
g_{cc} (μ_N)	+0.0244(4)
$2\chi_{aa} - \chi_{bb} - \chi_{cc}$	$18.3(5) \times 10^{-6} \text{ erg/G}^2 \cdot \text{mol}$
$-\chi_{aa} + 2\chi_{bb} - \chi_{cc}$	$14.9(6) \times 10^{-6} \text{ erg/G}^2 \cdot \text{mol}$

^aThe value of τ_3 is fixed by setting $R_6 = 0$.Table 25.2. Rotational constants for the ¹³C isotopic species of Methylene cyclopropane. [70062]

Parameter	¹³ CH ₂ CH ₂ CCH ₂	CH ₂ CH ₂ ¹³ CCH ₂	CH ₂ ¹³ CH ₂ CCH ₂
	A (MHz)	19424.(10)	19422.(10)
B (MHz)	6641.30(3)	6869.05(3)	6795.51(3)
C (MHz)	5296.18(3)	5440.07(3)	5360.78(3)

TABLE 25.3. Microwave spectrum of methylenecyclopropane

C₄H₆



Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
$\text{CH}_2\text{CCH}_2\text{CH}_2$ 	8585.980	(0.050)	3(1, 2) - 3(1, 3)	[70062]
	12090.430	(0.050)	7(2, 5) - 7(2, 6)	[70062]
	12322.307	(0.010)	1(0, 1) - 0(0, 0)	[70063]
	14278.707	(0.040)	4(1, 3) - 4(1, 4)	[70063]
	18487.390	(0.050)	8(2, 6) - 8(2, 7)	[70062]
	21316.600	(0.050)	5(1, 4) - 5(1, 5)	[70062]
	23212.478	(0.020)	2(1, 2) - 1(1, 1)	[70063]
	24528.790	(0.020)	2(0, 2) - 1(0, 1)	[70063]
	26076.420	(0.010)	2(1, 1) - 1(1, 0)	[70063]
	26350.970	(0.050)	9(2, 7) - 9(2, 8)	[70062]
	34749.020	(0.050)	3(1, 3) - 2(1, 2)	[70062]
	36508.560	(0.050)	3(0, 3) - 2(0, 2)	[70062]
	36966.320	(0.050)	3(2, 2) - 2(2, 1)	[70062]
	37424.430	(0.050)	3(2, 1) - 2(2, 0)	[70062]
	39039.020	(0.050)	3(1, 2) - 2(1, 1)	[70062]
¹³ CH ₂ CCH ₂ CH ₂ ¹³ C ₁	11937.540	(0.050)	1(0, 1) - 0(0, 0)	[70062]
	22529.840	(0.050)	2(1, 2) - 1(1, 1)	[70062]
	23774.300	(0.050)	2(0, 2) - 1(0, 1)	[70062]
CH ₂ ¹³ CCH ₂ CH ₂ ¹³ C ₂	25220.080	(0.050)	2(1, 1) - 1(1, 0)	[70062]
	12309.200	(0.050)	1(0, 1) - 0(0, 0)	[70062]
	23189.260	(0.050)	2(1, 2) - 1(1, 1)	[70062]
CH ₂ C ¹³ CH ₂ CH ₂ ¹³ C ₃	24503.060	(0.050)	2(0, 2) - 1(0, 1)	[70062]
	26047.220	(0.050)	2(1, 1) - 1(1, 0)	[70062]
	12156.350	(0.050)	1(0, 1) - 0(0, 0)	[70062]
$\text{CH}_2\text{C}^{13}\text{CH}_2\text{CH}_2$ ¹³ C ₃ 	12350.090	(0.050)	7(2, 5) - 7(2, 6)	[70062]
	18834.220	(0.050)	8(2, 6) - 8(2, 7)	[70062]
	22877.860	(0.050)	2(1, 2) - 1(1, 1)	[70062]
	24193.450	(0.050)	2(0, 2) - 1(0, 1)	[70062]
	25747.310	(0.050)	2(1, 1) - 1(1, 0)	[70062]
	26776.6	(0.2)	9(2, 7) - 9(2, 8)	[70062]

Table 26.1. Molecular constants for the ground vibrational state of cis- and skew-1-butene.

Parameter	cis-1-butene	skew-1-butene
<u>Rotational Constants</u> [present]		
A' (MHz)	15302.559(25)	22557.431(33)
B' (MHz)	5574.9560(64)	4156.123(13)
C' (MHz)	4303.1269(75)	4056.202(13)
τ_1 (MHz)	a	0.2425(66)
τ_2 (kHz)	-4.3111(4)	28.50(221)
τ_3 (MHz)	0.37(3)	6.86(150)
τ_{aaaa} (MHz)	-0.103(21)	a
τ_{bbbb} (kHz)	-21.528(804)	-8.422(2053)
τ_{cccc} (kHz)	-5.093(1009)	-15.033(2020)
<u>Electric Dipole Moment</u> [68043]		
μ_a (D)	0.368(4)	0.345(7)
μ_b (D)	0.237(6)	0.081(11)
μ_c (D)	---	0.059(16)

^aNot determinable.

Comments: An error in reference [68043] has been corrected. The $1_{11}-0_{00}$ transition frequency for skew-1-butene should be 26713.84 rather than 26613.84.

Table 26.2. Molecular constants for excited vibrational states of 1-butene. [68043]

Parameter	cis-1-butene	skew-1-butene
<u>CC torsion v=1</u>		
A (MHz)	15338.60	22545.89
B (MHz)	5539.25	4166.65
C (MHz)	4301.14	4068.25
<u>CC torsion v=2</u>		
A (MHz)	15392.70	22542.82 ^a 22543.99 ^a
B (MHz)	5516.67	4177.15
C (MHz)	4294.62	4078.45
<u>Methyl torsion v=1</u>		
A (MHz)	15274.57	22571.19
B (MHz)	5547.22	4150.52
C (MHz)	4290.53	4052.51
<u>Methyl torsion v=2</u>		
A (MHz)	15274.57	
B (MHz)	5519.95	
C (MHz)	4278.05	
<u>Skeletal bend v=1</u>		
B (MHz)		4148.85
C (MHz)		4043.08

^aThe two values refer to the doublet components for the $J(1,J-1) - J(0,J)$ transitions.

Table 26.3. Rotational constants for deuterated and ^{13}C isotopic forms of 1-butene.

Species ^a	Parameter	cis-1-butene	skew-1-butene	Reference
1-d	A (MHz)	15154.73	22159.8	[68043]
	B (MHz)	5197.01	3924.04	
	C (MHz)	4063.89	3823.00	
2-d	A (MHz)	14279.29	21083.7	[68043]
	B (MHz)	5518.02	4006.04	
	C (MHz)	4185.50	3924.16	
3-d	A (MHz)	14381.80	20477.	[68043]
	B (MHz)	5456.94	4108.80	
	C (MHz)	4159.06	4002.65	
4-d	A (MHz)	14261.64	20342.4	[68043]
	B (MHz)	5474.89	4113.03	
	C (MHz)	4207.41	3981.11	
5-d	A (MHz)		20592.9	[68043]
	B (MHz)		4143.13	
	C (MHz)		3993.69	
6-d	A (MHz)	15233.15		[68043]
	B (MHz)	5209.19	3925.09	
	C (MHz)	4077.42	3837.82	
7-d	A (MHz)	14367.82		[68043]
	B (MHz)	5441.16	4023.63	
	C (MHz)	4197.86	3902.19	
8-d	B (MHz)		4047.80	[68043]
	C (MHz)		3946.61	
1,1-d ₂	A (MHz)	14187.125(11)	20858.(200)	[81038]
	B (MHz)	5148.606(4)	3795.009(34)	[80033]
	C (MHz)	3962.463(4)	3710.571(34)	
1,3-d ₂	A (MHz)	14197.37	20173.	[68043]
	B (MHz)	5105.83	3880.38	
	C (MHz)	3937.88	3780.03	
2,3-d ₂	B (MHz)		3980.54	[68043]
	C (MHz)		3857.63	
4,5-d ₂	B (MHz)		4081.14	[68043]
	C (MHz)		3939.25	
4,6-d ₂	B (MHz)		3886.88	[68043]
	C (MHz)		3774.58	
4,7-d ₂	B (MHz)		3974.43	[68043]
	C (MHz)		3844.13	
4,8-d ₂	B (MHz)		4024.61	[68043]
	C (MHz)		3861.02	
5,6-d ₂	B (MHz)		3915.52	[68043]
	C (MHz)		3782.18	
5,7-d ₂	B (MHz)		4016.84	[68043]
	C (MHz)		3839.49	
5,8-d ₂	B (MHz)		4021.58	[68043]
	C (MHz)		3901.38	
d _n	A (MHz)	10597.801(8)		[81038]
	B (MHz)	4412.849(6)	3313.17	[79033]
	C (MHz)	3374.997(6)	3221.16	
1- ^{13}C	A (MHz)	15148.537(16)		[81038]
	B (MHz)	5442.077(3)	4044.66	[79033]
	C (MHz)	4211.638(3)	3952.64	
4- ^{13}C	B (MHz)		4053.72	[79033]
	C (MHz)		3956.64	

^aSee references [68043] and [79033] for hydrogen atom numbering.

Table 26.4. Centrifugal distortion constants for isotopic forms of 1-butene.

Parameter	cis-1,1-d ₂ [81038]	cis-1- ¹³ C [81038]	cis-d ₈ [81038]	skew-1,1d ₂ [80033]
Δ_J (kHz)	2.959(56)	3.37(6)	2.01(12)	3.13(24)
Δ_{JK} (kHz)	-7.94(32)	-9.90(27)	-4.16(15)	-53.89(72)
Δ_K (kHz)	24.8(12)	31.7(34)	11.6(10)	
δ_J (kHz)	0.888(25)	0.991(14)	0.590(10)	-0.82(40)
δ_K (kHz)	3.67(7)	4.15(36)	1.06(22)	

TABLE 26.5. Microwave spectrum of 1-butene

C₄H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_1	Sym.	Vib. state	Ref.	
c-CH ₂ CHCH ₂ CH ₃	9878.05	(0.10)	1(0, 1) - 0(0, 0)				[68043]	
	9911.79	(0.10)	2(0, 2) - 1(1, 1)				[68043]	
	10093.93	(0.10)	14(4, 10) - 14(4, 11)				[68043]	
	10999.38	(0.10)	1(1, 0) - 1(0, 1)				[68043]	
	12387.99	(0.10)	2(1, 1) - 2(0, 2)				[68043]	
	14186.07	(0.10)	11(3, 8) - 11(3, 9)				[68043]	
	14679.49	(0.10)	3(1, 2) - 3(0, 3)				[68043]	
	15550.86	(0.10)	15(4, 11) - 15(4, 12)				[68043]	
	16094.77	(0.10)	19(5, 14) - 19(5, 15)				[68043]	
	18080.54	(0.10)	4(1, 3) - 4(0, 4)				[68043]	
	18484.30	(0.10)	2(1, 2) - 1(1, 1)				[68043]	
	19605.70	(0.10)	1(1, 1) - 0(0, 0)				[68043]	
	19639.36	(0.10)	2(0, 2) - 1(0, 1)				[68043]	
	20600.76	(0.10)	3(0, 3) - 2(1, 2)				[68043]	
	21027.90	(0.10)	2(1, 1) - 1(1, 0)				[68043]	
	22762.12	(0.10)	5(1, 4) - 5(0, 5)				[68043]	
	23340.92	(0.10)	20(5, 15) - 20(5, 16)				[68043]	
	25890.90	(0.10)	5(2, 3) - 5(1, 4)				[68043]	
	25980.86	(0.10)	6(2, 4) - 6(1, 5)				[68043]	
	26661.14	(0.10)	4(2, 2) - 4(1, 3)				[68043]	
	27091.00	(0.10)	7(2, 5) - 7(1, 6)	2	E		[68043]	
	27093.92	(0.10)	7(2, 5) - 7(1, 6)	2	A		[68043]	
	27220.76	(0.10)	7(2, 5) - 7(1, 6)				[68043]	
	27464.68	(0.10)	3(1, 3) - 2(1, 2)	2	A		[68043]	
	27656.48	(0.10)	3(1, 3) - 2(1, 2)				[68043]	
	27928.88	(0.10)	3(2, 1) - 3(1, 2)				[68043]	
	28211.92	(0.10)	2(1, 2) - 1(0, 1)				[68043]	
	28266.80	(0.10)	6(1, 5) - 6(0, 6)	2	E		[68043]	
	28272.40	(0.10)	6(1, 5) - 6(0, 6)	2	A		[68043]	
	28763.56	(0.10)	6(1, 5) - 6(0, 6)				[68043]	
	28954.80	(0.10)	3(0, 3) - 2(0, 2)	2	E		[68043]	
	28955.50	(0.10)	3(0, 3) - 2(0, 2)	2	A		[68043]	
	29173.48	(0.10)	3(0, 3) - 2(0, 2)				[68043]	
	29299.48	(0.10)	2(2, 0) - 2(1, 1)				[68043]	
	29531.02	(0.10)	8(2, 6) - 8(1, 7)	2	E		[68043]	
	29535.12	(0.10)	8(2, 6) - 8(1, 7)	2	A		[68043]	
	29634.40	(0.10)	3(2, 2) - 2(2, 1)				[68043]	
	29830.44	(0.10)	8(2, 6) - 8(1, 7)				[68043]	
	30094.44	(0.10)	3(2, 1) - 2(2, 0)				[68043]	
	31180.46	(0.10)	17(4, 13) - 17(4, 14)				[68043]	
	31183.52	(0.10)	3(1, 2) - 2(1, 1)	2	E		[68043]	
	31184.88	(0.10)	3(1, 2) - 2(1, 1)	2	A		[68043]	
	31343.56	(0.10)	4(0, 4) - 3(1, 3)				[68043]	
	31465.02	(0.10)	3(1, 2) - 2(1, 1)				[68043]	
	33215.64	(0.10)	10(2, 8) - 10(2, 9)				[68043]	
	33442.80	(0.10)	9(2, 7) - 9(1, 8)	2	E		[68043]	
	33448.66	(0.10)	9(2, 7) - 9(1, 8)	2	A		[68043]	
	33958.86	(0.10)	9(2, 7) - 9(1, 8)				[68043]	
	34975.72	(0.10)	3(2, 2) - 3(1, 3)				[68043]	
	c- ¹³ CH ₂ CHCH ₂ CH ₃	8348.35	(0.10)	10(3, 7) - 10(3, 8)				[81038]
		9136.60	(0.10)	14(4, 10) - 14(4, 11)				[81038]
		9327.52	(0.10)	18(5, 13) - 18(5, 14)				[81038]
		9491.20	(0.10)	2(0, 2) - 1(1, 1)				[81038]
9653.70		(0.10)	1(0, 1) - 0(0, 0)				[81038]	
10936.87		(0.10)	1(1, 0) - 1(0, 1)				[81038]	
11112.32		(0.10)	7(2, 5) - 7(2, 6)				[81038]	
27049.63		(0.10)	3(1, 3) - 2(1, 2)				[81038]	
27783.45		(0.10)	2(1, 2) - 1(0, 1)				[81038]	
27888.53		(0.10)	3(2, 1) - 3(1, 2)				[81038]	
28035.05		(0.10)	6(1, 5) - 6(0, 6)				[81038]	
28527.62		(0.10)	3(0, 3) - 2(0, 2)				[81038]	
28961.00		(0.10)	3(2, 2) - 2(2, 1)				[81038]	
29325.20		(0.10)	8(2, 6) - 8(1, 7)				[81038]	
29394.13		(0.10)	3(2, 1) - 2(2, 0)				[81038]	
30734.48		(0.10)	3(1, 2) - 2(1, 1)				[81038]	
32810.35		(0.10)	2(2, 1) - 2(1, 2)				[81038]	
33181.15		(0.10)	9(2, 7) - 9(1, 8)				[81038]	

TABLE 26.5. Microwave spectrum of 1-butene — Continued

C₄H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_1	Sym.	Vib. state	Ref.
	34721.80	(0.10)	3(2, 2) - 3(1, 3)				[81038]
	35635.38	(0.10)	3(1, 3) - 2(0, 2)				[81038]
	35931.38	(0.10)	4(1, 4) - 3(1, 3)				[81038]
	37299.28	(0.10)	4(2, 3) - 4(1, 4)				[81038]
	37873.70	(0.10)	8(2, 6) - 7(3, 5)				[81038]
	38290.50	(0.10)	6(1, 5) - 5(2, 4)				[81038]
	38528.83	(0.10)	4(2, 3) - 3(2, 2)				[81038]
	38548.10	(0.10)	10(2, 8) - 10(1, 9)				[81038]
	38816.85	(0.10)	4(3, 2) - 3(3, 1)				[81038]
	38853.47	(0.10)	4(3, 1) - 3(3, 0)				[81038]
	39152.77	(0.10)	11(3, 8) - 11(2, 9)				[81038]
	39271.28	(0.10)	10(3, 7) - 10(2, 8)				[81038]
	39576.70	(0.10)	4(2, 2) - 3(2, 1)				[81038]
<i>c</i> -CD ₂ CDCD ₂ CD ₃	27002.65	(0.10)	3(1, 3) - 2(0, 2)				[81038]
	27181.95	(0.10)	11(3, 8) - 11(2, 9)				[81038]
	27572.00	(0.10)	7(3, 4) - 7(2, 5)				[81038]
	28074.08	(0.10)	7(1, 6) - 7(0, 7)				[81038]
	28264.02	(0.10)	5(2, 4) - 5(1, 5)				[81038]
	28859.47	(0.10)	4(1, 4) - 3(1, 3)				[81038]
	29347.10	(0.10)	6(3, 3) - 6(2, 4)				[81038]
	30036.83	(0.10)	4(0, 4) - 3(0, 3)				[81038]
	30207.20	(0.10)	12(3, 9) - 12(2, 10)				[81038]
	31004.85	(0.10)	5(3, 2) - 5(2, 3)				[81038]
	31057.40	(0.10)	4(2, 3) - 3(2, 2)				[81038]
	31367.07	(0.10)	4(3, 2) - 3(3, 1)				[81038]
	31418.97	(0.10)	4(3, 1) - 3(3, 0)				[81038]
	31587.97	(0.10)	6(2, 5) - 6(1, 6)				[81038]
	31664.25	(0.10)	10(2, 8) - 10(1, 9)				[81038]
	32170.90	(0.10)	4(2, 2) - 3(2, 1)				[81038]
	32257.33	(0.10)	4(3, 1) - 4(2, 2)				[81038]
	32958.59	(0.10)	4(1, 3) - 3(1, 2)				[81038]
	32968.35	(0.10)	4(1, 4) - 3(0, 3)				[81038]
	33511.55	(0.10)	14(4, 10) - 14(3, 11)				[81038]
	33553.80	(0.10)	13(4, 9) - 13(3, 10)				[81038]
	33899.62	(0.10)	4(3, 2) - 4(2, 3)				[81038]
	33976.66	(0.10)	5(0, 5) - 4(1, 4)				[81038]
	34494.67	(0.10)	5(3, 3) - 5(2, 4)				[81038]
	34677.32	(0.10)	13(3, 10) - 13(2, 11)				[81038]
	34817.07	(0.10)	12(4, 8) - 12(3, 9)				[81038]
	34956.13	(0.10)	15(4, 11) - 15(3, 12)				[81038]
	35168.25	(0.10)	2(2, 1) - 1(1, 0)				[81038]
	35424.07	(0.10)	7(2, 6) - 7(1, 7)				[81038]
	35473.48	(0.10)	6(3, 4) - 6(2, 5)				[81038]
	35697.43	(0.10)	6(1, 5) - 5(2, 4)				[81038]
	35902.22	(0.10)	5(1, 5) - 4(1, 4)				[81038]
	36326.15	(0.10)	2(2, 0) - 1(1, 1)				[81038]
	36908.17	(0.10)	5(0, 5) - 4(0, 4)				[81038]
	36912.95	(0.10)	11(4, 7) - 11(3, 8)				[81038]
	36921.52	(0.10)	7(3, 5) - 7(2, 6)				[81038]
	38021.70	(0.10)	16(4, 12) - 16(3, 13)				[81038]
	38672.17	(0.10)	5(2, 4) - 4(2, 3)				[81038]
	38833.72	(0.10)	5(1, 5) - 4(0, 4)				[81038]
	39267.18	(0.10)	5(3, 3) - 4(3, 2)				[81038]
	39445.56	(0.10)	5(3, 2) - 4(3, 1)				[81038]
<i>c</i> -CD ₂ CHCH ₂ CH ₃	8459.65	(0.10)	10(3, 7) - 10(3, 8)				[81038]
	9111.25	(0.10)	1(0, 1) - 0(0, 0)				[81038]
	9496.05	(0.10)	14(4, 10) - 14(4, 11)				[81038]
	9951.02	(0.10)	18(5, 13) - 18(5, 14)				[81038]
	10224.70	(0.10)	1(1, 0) - 1(0, 1)				[81038]
	10949.15	(0.10)	7(2, 5) - 7(2, 6)				[81038]
	11520.25	(0.10)	2(1, 1) - 2(0, 2)				[81038]
	11818.55	(0.10)	4(1, 3) - 4(1, 4)				[81038]
	27224.10	(0.10)	2(2, 0) - 2(1, 1)				[81038]
	27333.75	(0.10)	3(2, 2) - 2(2, 1)				[81038]
	27764.72	(0.10)	3(2, 1) - 2(2, 0)				[81038]
	27770.48	(0.10)	8(2, 6) - 8(1, 7)				[81038]
	28855.65	(0.10)	4(0, 4) - 3(1, 3)				[81038]

TABLE 26.5. Microwave spectrum of 1-butene — Continued

C₄H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_1	Sym.	Vib. state	Ref.
	29004.15	(0.10)	12(4, 8) - 11(5, 7)				[81038]
	29041.18	(0.10)	3(1, 2) - 2(1, 1)				[81038]
	30673.70	(0.10)	2(2, 1) - 2(1, 2)				[81038]
	31638.40	(0.10)	9(2, 7) - 9(1, 8)				[81038]
	32518.65	(0.10)	3(2, 2) - 3(1, 3)				[81038]
	32760.00	(0.10)	10(3, 7) - 9(4, 6)				[81038]
	33450.07	(0.10)	3(1, 3) - 2(0, 2)				[81038]
	33871.12	(0.10)	4(1, 4) - 3(1, 3)				[81038]
	35006.90	(0.10)	4(2, 3) - 4(1, 4)				[81038]
	35403.32	(0.10)	4(0, 4) - 3(0, 3)				[81038]
	35833.15	(0.10)	17(6,11) - 16(7,10)				[81038]
	36359.41	(0.10)	4(2, 3) - 3(2, 2)				[81038]
	36528.65	(0.10)	10(3, 7) - 10(2, 8)				[81038]
	36641.55	(0.10)	6(1, 5) - 5(2, 4)				[81038]
	36643.27	(0.10)	11(3, 8) - 11(2, 9)				[81038]
	36645.70	(0.10)	4(3, 2) - 3(3, 1)				[81038]
	36683.38	(0.10)	4(3, 1) - 3(3, 0)				[81038]
	36722.30	(0.10)	8(2, 6) - 7(3, 5)				[81038]
	37400.18	(0.10)	4(2, 2) - 3(2, 1)				[81038]
	37584.08	(0.10)	9(3, 6) - 9(2, 7)				[81038]
	38146.40	(0.10)	5(2, 4) - 5(1, 5)				[81038]
	38194.23	(0.10)	12(3, 9) - 12(2,10)				[81038]
	38578.33	(0.10)	4(1, 3) - 3(1, 2)				[81038]
	38587.72	(0.10)	5(0, 5) - 4(1, 4)				[81038]
	39448.42	(0.10)	8(3, 5) - 8(2, 6)				[81038]
s-CH ₂ CHCH ₂ CH ₃	8212.46	(0.10)	1(0, 1) - 0(0, 0)				[68043]
	13181.66	(0.10)	15(1,15) - 15(0,15)				[68043]
	13190.73	(0.10)	15(1,15) - 15(0,15)	0	A	2ν ₁	[68043]
	13200.86	(0.10)	15(1,15) - 15(0,15)	0	E	2ν ₁	[68043]
	13230.51	(0.10)	15(1,15) - 15(0,15)	0	A	1ν ₁	[68043]
	13230.87	(0.10)	15(1,15) - 15(0,15)	0	E	1ν ₁	[68043]
	13763.28	(0.10)	14(1,14) - 14(0,14)				[68043]
	13766.70	(0.10)	14(1,14) - 14(0,14)	0	A	2ν ₁	[68043]
	13776.69	(0.10)	14(1,14) - 14(0,14)	0	E	2ν ₁	[68043]
	13805.03	(0.10)	14(1,14) - 14(0,14)	0	A	1ν ₁	[68043]
	13805.40	(0.10)	14(1,14) - 14(0,14)	0	E	1ν ₁	[68043]
	14323.54	(0.10)	13(1,13) - 13(0,13)	0	A	2ν ₁	[68043]
	14325.69	(0.10)	13(1,13) - 13(0,13)				[68043]
	14333.51	(0.10)	13(1,13) - 13(0,13)	0	E	2ν ₁	[68043]
	14360.38	(0.10)	13(1,13) - 13(0,13)	0	A	1ν ₁	[68043]
	14360.75	(0.10)	13(1,13) - 13(0,13)	0	E	1ν ₁	[68043]
	14857.60	(0.10)	12(1,12) - 12(0,12)	0	A,E	2ν ₁	[68043]
	14864.97	(0.10)	12(1,12) - 12(0,12)				[68043]
	14892.71	(0.10)	12(1,12) - 12(0,12)	0	A	1ν ₁	[68043]
	14893.03	(0.10)	12(1,12) - 12(0,12)	0	E	1ν ₁	[68043]
	15365.11	(0.10)	11(1,11) - 11(0,11)	0	A	2ν ₁	[68043]
	15374.89	(0.10)	11(1,11) - 11(0,11)	0	E	2ν ₁	[68043]
	15377.58	(0.10)	11(1,11) - 11(0,11)				[68043]
	15398.38	(0.10)	11(1,11) - 11(0,11)	0	A	1ν ₁	[68043]
	15398.74	(0.10)	11(1,11) - 11(0,11)	0	E	1ν ₁	[68043]
	15842.62	(0.10)	10(1,10) - 10(0,10)	0	A	2ν ₁	[68043]
	15852.50	(0.10)	10(1,10) - 10(0,10)	0	E	2ν ₁	[68043]
	15859.89	(0.10)	10(1,10) - 10(0,10)				[68043]
	15874.13	(0.10)	10(1,10) - 10(0,10)	0	A	1ν ₁	[68043]
	15874.48	(0.10)	10(1,10) - 10(0,10)	0	E	1ν ₁	[68043]
	16307.89	(0.10)	2(1, 2) - 1(1, 1)	1	A		[68043]
	16308.17	(0.10)	2(1, 2) - 1(1, 1)	1	E		[68043]
	16325.14	(0.10)	2(1, 2) - 1(1, 1)				[68043]
	16424.43	(0.10)	2(0, 2) - 1(0, 1)				[68043]
	16503.95	(0.10)	2(1, 1) - 1(1, 0)	1	E		[68043]
	16504.15	(0.10)	2(1, 1) - 1(1, 0)	1	A		[68043]
	16525.00	(0.10)	2(1, 1) - 1(1, 0)				[68043]
	16695.60	(0.10)	8(1, 8) - 8(0, 8)	0	A	2ν ₁	[68043]
	16705.22	(0.10)	8(1, 8) - 8(0, 8)	0	E	2ν ₁	[68043]
	16721.29	(0.10)	8(1, 8) - 8(0, 8)				[68043]
	16723.28	(0.10)	8(1, 8) - 8(0, 8)	0	A	1ν ₁	[68043]
	16723.62	(0.10)	8(1, 8) - 8(0, 8)	0	E	1ν ₁	[68043]

TABLE 26.5. Microwave spectrum of 1-butene — Continued

C₄H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_1	Sym.	Vib. state	Ref.
	17065.04	(0.10)	7(1, 7) - 7(0, 7)	0	A	2 ν_1	[68043]
	17074.78	(0.10)	7(1, 7) - 7(0, 7)	0	E	2 ν_1	[68043]
	17091.24	(0.10)	7(1, 7) - 7(0, 7)	0	A	1 ν_1	[68043]
	17091.54	(0.10)	7(1, 7) - 7(0, 7)	0	E	1 ν_1	[68043]
	17094.62	(0.10)	7(1, 7) - 7(0, 7)	0			[68043]
	17393.78	(0.10)	6(1, 6) - 6(0, 6)	0	A	2 ν_1	[68043]
	17403.40	(0.10)	6(1, 6) - 6(0, 6)	0	E	2 ν_1	[68043]
	17418.20	(0.10)	6(1, 6) - 6(0, 6)	0	A	1 ν_1	[68043]
	17418.60	(0.10)	6(1, 6) - 6(0, 6)	0	E	1 ν_1	[68043]
	17426.56	(0.10)	6(1, 6) - 6(0, 6)	0			[68043]
	17679.56	(0.10)	5(1, 5) - 5(0, 5)	0	A	2 ν_1	[68043]
	17688.86	(0.10)	5(1, 5) - 5(0, 5)	0	E	2 ν_1	[68043]
	17702.40	(0.10)	5(1, 5) - 5(0, 5)	0	A	1 ν_1	[68043]
	17702.70	(0.10)	5(1, 5) - 5(0, 5)	0	E	1 ν_1	[68043]
	17714.77	(0.10)	5(1, 5) - 5(0, 5)	0			[68043]
	17919.40	(0.10)	4(1, 4) - 4(0, 4)	0	A	2 ν_1	[68043]
	17928.80	(0.10)	4(1, 4) - 4(0, 4)	0	E	2 ν_1	[68043]
	17957.80	(0.10)	4(1, 4) - 4(0, 4)	0			[68043]
	18113.60	(0.10)	3(1, 3) - 3(0, 3)	0	A,E	2 ν_1	[68043]
	18153.93	(0.10)	3(1, 3) - 3(0, 3)	0			[68043]
	18302.10	(0.10)	2(1, 2) - 2(0, 2)	0			[68043]
	18401.20	(0.10)	1(1, 1) - 1(0, 1)	0			[68043]
	18501.28	(0.10)	1(1, 0) - 1(0, 1)	0			[68043]
	18601.64	(0.10)	2(1, 1) - 2(0, 2)	0			[68043]
	18712.42	(0.10)	3(1, 2) - 3(0, 3)	0	A	2 ν_1	[68043]
	18713.66	(0.10)	3(1, 2) - 3(0, 3)	0	E	2 ν_1	[68043]
	18725.60	(0.10)	3(1, 2) - 3(0, 3)	0	A,E	1 ν_1	[68043]
	18753.00	(0.10)	3(1, 2) - 3(0, 3)	0			[68043]
	18764.62	(0.10)	3(1, 2) - 3(0, 3)	1	A		[68043]
	18766.22	(0.10)	3(1, 2) - 3(0, 3)	1	E		[68043]
	18914.20	(0.10)	4(1, 3) - 4(0, 4)	0	A	2 ν_1	[68043]
	18915.30	(0.10)	4(1, 3) - 4(0, 4)	0	E	2 ν_1	[68043]
	18926.10	(0.10)	4(1, 3) - 4(0, 4)	0	A,E	1 ν_1	[68043]
	18957.26	(0.10)	4(1, 3) - 4(0, 4)	0			[68043]
	18964.72	(0.10)	4(1, 3) - 4(0, 4)	1	A		[68043]
	18966.26	(0.10)	4(1, 3) - 4(0, 4)	1	E		[68043]
	19168.80	(0.10)	5(1, 4) - 5(0, 5)	0	A	2 ν_1	[68043]
	19169.92	(0.10)	5(1, 4) - 5(0, 5)	0	E	2 ν_1	[68043]
	19179.42	(0.10)	5(1, 4) - 5(0, 5)	0	A,E	1 ν_1	[68043]
	19214.20	(0.10)	5(1, 4) - 5(0, 5)	0			[68043]
	19217.24	(0.10)	5(1, 4) - 5(0, 5)	1	A		[68043]
	19218.86	(0.10)	5(1, 4) - 5(0, 5)	1	E		[68043]
	19477.53	(0.10)	6(1, 5) - 6(0, 6)	0	A	2 ν_1	[68043]
	19478.67	(0.10)	6(1, 5) - 6(0, 6)	0	E	2 ν_1	[68043]
	19486.46	(0.10)	6(1, 5) - 6(0, 6)	0	A,E	1 ν_1	[68043]
	19523.06	(0.10)	6(1, 5) - 6(0, 6)	1	A		[68043]
	19524.62	(0.10)	6(1, 5) - 6(0, 6)	1	E		[68043]
	19526.14	(0.10)	6(1, 5) - 6(0, 6)	0			[68043]
	19842.45	(0.10)	7(1, 6) - 7(0, 7)	0	A	2 ν_1	[68043]
	19843.61	(0.10)	7(1, 6) - 7(0, 7)	0	E	2 ν_1	[68043]
	19849.20	(0.10)	7(1, 6) - 7(0, 7)	0	A,E	1 ν_1	[68043]
	19884.73	(0.10)	7(1, 6) - 7(0, 7)	1	A		[68043]
	19886.41	(0.10)	7(1, 6) - 7(0, 7)	1	E		[68043]
	19894.69	(0.10)	7(1, 6) - 7(0, 7)	0			[68043]
	20265.59	(0.10)	8(1, 7) - 8(0, 8)	0	A	2 ν_1	[68043]
	20266.70	(0.10)	8(1, 7) - 8(0, 8)	0	E	2 ν_1	[68043]
	20269.88	(0.10)	8(1, 7) - 8(0, 8)	0	A,E	1 ν_1	[68043]
	20304.14	(0.10)	8(1, 7) - 8(0, 8)	1	A		[68043]
	20305.92	(0.10)	8(1, 7) - 8(0, 8)	1	E		[68043]
	20322.18	(0.10)	8(1, 7) - 8(0, 8)	0			[68043]
	20749.27	(0.10)	9(1, 8) - 9(0, 9)	0	A	2 ν_1	[68043]
	20750.38	(0.10)	9(1, 8) - 9(0, 9)	0	E	2 ν_1	[68043]
	20750.84	(0.10)	9(1, 8) - 9(0, 9)	0	A,E	1 ν_1	[68043]
	20783.64	(0.10)	9(1, 8) - 9(0, 9)	1	A		[68043]
	20785.47	(0.10)	9(1, 8) - 9(0, 9)	1	E		[68043]
	20811.02	(0.10)	9(1, 8) - 9(0, 9)	0			[68043]
	21294.66	(0.10)	10(1, 9) - 10(0, 10)	0	A,E	1 ν_1	[68043]

TABLE 26.5. Microwave spectrum of 1-butene — Continued

C₄H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_1	Sym.	Vib. state	Ref.
	21296.28	(0.10)	10(1, 9) - 10(0, 10)	0	A	2 ν_1	[68043]
	21297.42	(0.10)	10(1, 9) - 10(0, 10)	0	E	2 ν_1	[68043]
	21325.93	(0.10)	10(1, 9) - 10(0, 10)	1	A		[68043]
	21327.87	(0.10)	10(1, 9) - 10(0, 10)	1	E		[68043]
	21363.88	(0.10)	10(1, 9) - 10(0, 10)				[68043]
	21904.18	(0.10)	11(1, 10) - 11(0, 11)	0	A,E	1 ν_1	[68043]
	21909.25	(0.10)	11(1, 10) - 11(0, 11)	0	A	2 ν_1	[68043]
	21910.41	(0.10)	11(1, 10) - 11(0, 11)	0	E	2 ν_1	[68043]
	21933.64	(0.10)	11(1, 10) - 11(0, 11)	1	A		[68043]
	21935.76	(0.10)	11(1, 10) - 11(0, 11)	1	E		[68043]
	21983.88	(0.10)	11(1, 10) - 11(0, 11)				[68043]
	22582.60	(0.10)	12(1, 11) - 12(0, 12)	0	A,E	1 ν_1	[68043]
	22591.36	(0.10)	12(1, 11) - 12(0, 12)	0	A	2 ν_1	[68043]
	22592.61	(0.10)	12(1, 11) - 12(0, 12)	0	E	2 ν_1	[68043]
	22610.08	(0.10)	12(1, 11) - 12(0, 12)	1	A		[68043]
	22612.34	(0.10)	12(1, 11) - 12(0, 12)	1	E		[68043]
	22674.14	(0.10)	12(1, 11) - 12(0, 12)				[68043]
	23334.00	(0.10)	13(1, 12) - 13(0, 13)	0	A,E	1 ν_1	[68043]
	23346.40	(0.10)	13(1, 12) - 13(0, 13)	0	A	2 ν_1	[68043]
	23347.60	(0.10)	13(1, 12) - 13(0, 13)	0	E	2 ν_1	[68043]
	23438.14	(0.10)	13(1, 12) - 13(0, 13)				[68043]
	24160.00	(0.10)	14(1, 13) - 14(0, 14)	0	A,E	1 ν_1	[68043]
	24177.20	(0.10)	14(1, 13) - 14(0, 14)	0	A	2 ν_1	[68043]
	24178.40	(0.10)	14(1, 13) - 14(0, 14)	0	E	2 ν_1	[68043]
	24279.38	(0.10)	14(1, 13) - 14(0, 14)				[68043]
	24461.32	(0.10)	3(1, 3) - 2(1, 2)	1	A		[68043]
	24461.46	(0.10)	3(1, 3) - 2(1, 2)	1	E		[68043]
	24487.28	(0.10)	3(1, 3) - 2(1, 2)				[68043]
	24635.40	(0.10)	3(0, 3) - 2(0, 2)				[68043]
	24638.82	(0.10)	3(2, 2) - 2(2, 1)				[68043]
	24640.00	(0.10)	3(2, 1) - 2(2, 0)				[68043]
	24755.84	(0.10)	3(1, 2) - 2(1, 1)	1	A		[68043]
	24755.88	(0.10)	3(1, 2) - 2(1, 1)	1	E		[68043]
	24787.28	(0.10)	3(1, 2) - 2(1, 1)				[68043]
	25065.28	(0.10)	15(1, 14) - 15(0, 15)	0	A,E	1 ν_1	[68043]
	25087.42	(0.10)	15(1, 14) - 15(0, 15)	0	A	2 ν_1	[68043]
	25088.60	(0.10)	15(1, 14) - 15(0, 15)	0	E	2 ν_1	[68043]
	25201.76	(0.10)	15(1, 14) - 15(0, 15)				[68043]
	26713.84	(0.10)	1(1, 0) - 0(0, 0)				[68043]
	32648.84	(0.10)	4(1, 4) - 3(1, 3)				[68043]
	32845.10	(0.10)	4(0, 4) - 3(0, 3)				[68043]
	32851.26	(0.10)	4(2, 3) - 3(2, 2)				[68043]
	32854.16	(0.10)	4(2, 2) - 3(2, 1)				[68043]
	33048.66	(0.10)	4(1, 3) - 3(1, 2)				[68043]
	34726.46	(0.10)	2(1, 2) - 1(0, 1)				[68043]
s- ¹³ CH ₂ CHCH ₂ CH ₃	23853.35	(0.10)	3(1, 3) - 2(1, 2)				[79033]
	23990.28	(0.10)	3(0, 3) - 2(0, 2)				[79033]
	23993.38	(0.10)	3(2, 2) - 2(2, 1)				[79033]
	23994.58	(0.10)	3(2, 1) - 2(2, 0)				[79033]
	24130.42	(0.10)	3(1, 2) - 2(1, 1)				[79033]
	31803.64	(0.10)	4(1, 4) - 3(1, 3)				[79033]
	31985.14	(0.10)	4(0, 4) - 3(0, 3)				[79033]
	31990.41	(0.10)	4(2, 3) - 3(2, 2)				[79033]
	31993.88	(0.10)	4(2, 2) - 3(2, 1)				[79033]
	32173.18	(0.10)	4(1, 3) - 3(1, 2)				[79033]
	39753.19	(0.10)	5(1, 5) - 4(1, 4)				[79033]
	39987.00	(0.10)	5(2, 4) - 4(2, 3)				[79033]
	39992.20	(0.10)	5(3, 2) - 4(3, 1)				[79033]
	39993.88	(0.10)	5(4, 1) - 4(4, 0)				[79033]
s-CH ₂ CHCH ₂ ¹³ CH ₃	39996.34	(0.10)	5(2, 3) - 4(2, 2)				[79033]
	24029.00	(0.10)	3(0, 3) - 2(0, 2)				[79033]
	31846.12	(0.10)	4(1, 4) - 3(1, 3)				[79033]
	32042.39	(0.10)	4(2, 3) - 3(2, 2)				[79033]
	32046.07	(0.10)	4(3, 1) - 3(3, 0)				[79033]
	32046.30	(0.10)	4(2, 2) - 3(2, 1)				[79033]
	32234.37	(0.10)	4(1, 3) - 3(1, 2)				[79033]
	39806.18	(0.10)	5(1, 5) - 4(1, 4)				[79033]

TABLE 26.5. Microwave spectrum of 1-butene — Continued

C₄H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_1	Sym.	Vib. state	Ref.
s-CD ₂ CDCD ₂ CD ₃	40051.75	(0.10)	5(2, 4) - 4(2, 3)				[79033]
	40057.27	(0.10)	5(3, 2) - 4(3, 1)				[79033]
	40059.75	(0.10)	5(2, 3) - 4(2, 2)				[79033]
	40061.45	(0.10)	5(4, 1) - 4(4, 0)				[79033]
	19464.66	(0.10)	3(1, 3) - 2(1, 2)				[79033]
	19600.62	(0.10)	3(0, 3) - 2(0, 2)				[79033]
	19603.49	(0.10)	3(2, 2) - 2(2, 1)				[79033]
	19605.74	(0.10)	3(2, 1) - 2(2, 0)				[79033]
	19740.73	(0.10)	3(1, 2) - 2(1, 1)				[79033]
	25951.90	(0.10)	4(1, 4) - 3(1, 3)				[79033]
	26137.30	(0.10)	4(2, 3) - 3(2, 2)				[79033]
	26139.77	(0.10)	4(3, 1) - 3(3, 0)				[79033]
	26139.77	(0.10)	4(3, 2) - 3(3, 1)				[79033]
	26142.96	(0.10)	4(2, 2) - 3(2, 1)				[79033]
	26320.14	(0.10)	4(1, 3) - 3(1, 2)				[79033]
	32438.35	(0.10)	5(1, 5) - 4(1, 4)				[79033]
	32659.39	(0.10)	5(0, 5) - 4(0, 4)				[79033]
	32670.52	(0.10)	5(2, 4) - 4(2, 3)				[79033]
	32674.86	(0.10)	5(3, 3) - 4(3, 2)				[79033]
	32674.86	(0.10)	5(3, 2) - 4(3, 1)				[79033]
	32675.77	(0.10)	5(4, 2) - 4(4, 1)				[79033]
	32675.77	(0.10)	5(4, 1) - 4(4, 0)				[79033]
	32681.92	(0.10)	5(2, 3) - 4(2, 2)				[79033]
	32898.79	(0.10)	5(1, 4) - 4(1, 3)				[79033]
	38923.76	(0.10)	6(1, 6) - 5(1, 5)				[79033]
	39203.02	(0.10)	6(2, 5) - 5(2, 4)				[79033]
	39210.08	(0.10)	6(3, 4) - 5(3, 3)				[79033]
	39210.08	(0.10)	6(3, 3) - 5(3, 2)				[79033]
	39210.77	(0.10)	6(4, 2) - 5(4, 1)				[79033]
	39210.77	(0.10)	6(4, 3) - 5(4, 2)				[79033]
	39212.73	(0.10)	6(5, 2) - 5(5, 1)				[79033]
	39212.73	(0.10)	6(5, 1) - 5(5, 0)				[79033]
	39222.98	(0.10)	6(2, 4) - 5(2, 3)				[79033]
39476.48	(0.10)	6(1, 5) - 5(1, 4)				[79033]	
s-CD ₂ CHCD ₂ CD ₃	32781.60	(0.10)	5(1, 5) - 4(1, 4)				[79033]
	36335.90	(0.10)	6(1, 6) - 5(1, 5)				[79033]
	39896.20	(0.10)	6(1, 5) - 5(1, 4)				[79033]
s-CD ₂ CHCH ₂ CH ₃	22389.78	(0.10)	3(1, 3) - 2(1, 2)				[80033]
	22515.22	(0.10)	3(0, 3) - 2(0, 2)				[80033]
	22517.80	(0.10)	3(2, 2) - 2(2, 1)				[80033]
	22518.85	(0.10)	3(2, 1) - 2(2, 0)				[80033]
	22643.26	(0.10)	3(1, 2) - 2(1, 1)				[80033]
	29852.23	(0.10)	4(1, 4) - 3(1, 3)				[80033]
	30018.38	(0.10)	4(0, 4) - 3(0, 3)				[80033]
	30023.02	(0.10)	4(2, 3) - 3(2, 2)				[80033]
	30026.05	(0.10)	4(2, 2) - 3(2, 1)				[80033]
	30026.05	(0.10)	4(3, 1) - 3(3, 0)				[80033]
	30190.42	(0.10)	4(1, 3) - 3(1, 2)				[80033]
	37314.02	(0.10)	5(1, 5) - 4(1, 4)				[80033]
	37520.02	(0.10)	5(0, 5) - 4(0, 4)				[80033]
	37527.81	(0.10)	5(2, 4) - 4(2, 3)				[80033]
	37532.70	(0.10)	5(3, 3) - 4(3, 2)				[80033]
	37532.70	(0.10)	5(3, 2) - 4(3, 1)				[80033]
	37534.09	(0.10)	5(2, 3) - 4(2, 2)				[80033]
	37535.64	(0.10)	5(4, 1) - 4(4, 0)				[80033]
	37737.01	(0.10)	5(1, 4) - 4(1, 3)				[80033]

Table 27.1. Molecular constants for *cis*-2-butene in the ground state.

Parameter Reference	CH ₃ CHCHCH ₃ [70067]	Parameter	CH ₃ CHCHCH ₃ [68049]
<u>Rotational Constants</u>			
	<u>A₁A₁ State</u>		<u>Rigid Rotor</u> <u>A₁A₁ State</u>
A (MHz)	16086.12	A (MHz)	16059.61 16085.76
B (MHz)	5144.33	B (MHz)	5139.15 5144.61
C (MHz)	4087.93	C (MHz)	4088.16 4088.16
<u>Internal Rotation Constants</u>			
I _α (u Å ²)	3.130	I _α (u Å ²)	3.194 ^a
λ _a	0.5850(12)	θ	35.0° ^a
λ _b	0.8111(9)	α	0.058199 ^b
r	0.94504		
q	0.0131	β	0.026598 ^b
s	20.39(11)	s	20.332
F (GHz)	170.937	F (GHz)	167.54
V ₃ (cm ⁻¹)	261.7(14)	V ₃ (cm ⁻¹)	255.8
<u>Electric Dipole Moment</u>			
μ _b (D)	0.253(5)	μ _b (D)	0.257(10)

^aAssumed.^bThe values are defined as $\alpha = (I_{\alpha}/I_a) \sin\theta$, $\beta = (I_{\alpha}/I_b) \cos\theta$.Comments: The 7¹⁶-7⁰⁷ transition reported at 31829.11 MHz deviates by about 3 MHz in the analysis and was not fit.

Table 27.2. Molecular constants for sym-CH₂DCHCHCH₃,
asy-CH₂DCHCHCH₃ and CH₃CDCDCH₃. [70067]

Parameter	sym-CH ₂ DCHCHCH ₃ Value	asy-CH ₂ DCHCHCH ₃ Value	CH ₃ CDCDCH ₃ Value
<u>Rotational Constants</u>			
A-C (A ₁) (MHz)	11040.37	11681.12	10033.99
B-C (A ₁) (MHz)	1101.06	938.69	1155.42
A-C (A ₂) (MHz)		11672.24	
B-C (A ₂) (MHz)		937.77	
<u>Internal Rotation Constants^a</u>			
λ _a	0.5538(16)	0.5684(28)	0.5883(54)
λ _b	0.8259(12)	0.8228(20) ^b	0.8086(39)
I _α (u Å ²)	3.130	3.130	3.130
r	0.94904	0.94823	0.95002
F (GHz)	170.184	170.329	170.026
s	20.42(2)	20.66(4)	20.96(7)
V ₃ (cm ⁻¹)	260.9(3)	264.2(5)	267.6(9)

^aValues with no uncertainties are calculated.^bA value for λ_c = 0.0034 was included.

Table 27.3. Molecular constants for $\text{CH}_3\text{CDCHCH}_3$. [70067]

Parameter	Value	
<u>Rotational Constants</u>		
A-C (A_1A_1) (MHz)	10942.28	
B-C (A_1A_1) (MHz)	1107.63	
<u>Internal Rotation Constants^a</u>		
	<u>A_1 State</u>	<u>A_2 State</u>
λ_a	-0.5700(164)	0.6118(124)
λ_b	0.8216(114)	0.7910(96)
I_α ($\text{u } \text{Å}^2$)	3.130	3.130
r	0.94883	0.94883
q	0.01178	0.01178
F (GHz)	170.248	170.789
s	20.68(11)	20.61(11)
x	-0.01245	
V_3 (cm^{-1})	264.4(14)	264.4(14)

^aValues without uncertainties are calculated.

Table 27.4. Molecular constants for d_8 and d_6 cis-2-butene. [79039]

Parameter	$\text{CD}_3\text{CD}_2\text{CD}_2$	$\text{CD}_3\text{CHCHCD}_2$
<u>Rotational Constants</u>		
A (MHz)	11136.1(3)	12684.2(2)
B (MHz)	3997.05(14)	4008.11(4)
C (MHz)	3170.96(11)	3346.45(4)
<u>Internal Rotation Constants</u>		
I_α ($\text{u } \text{Å}^2$)	5.83(20)	5.98(20)
θ	54.08(12)	54.27(1)
s	40.34(10)	39.31(8)
V_3 (cm^{-1})	284.(11)	272.(11)

TABLE 27.5. Microwave spectrum of cis-2-butene

C₄H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Sym.	Ref.	
c-CH ₃ CHCHCH ₃	20014.47	(0.20)	1(1, 1) - 0(0, 0)	EA	[68049]	
	20122.01	(0.20)	1(1, 1) - 0(0, 0)	EE	[68049]	
	20134.69	(0.20)	1(1, 1) - 0(0, 0)	AE	[68049]	
	20173.92	(0.20)	1(1, 1) - 0(0, 0)	AA	[68049]	
	21165.48	(0.20)	5(1, 4) - 5(0, 5)	EA	[68049]	
	21172.39	(0.20)	5(1, 4) - 5(0, 5)	AE	[68049]	
	21219.83	(0.20)	5(1, 4) - 5(0, 5)	EE	[68049]	
	21270.86	(0.20)	5(1, 4) - 5(0, 5)	AA	[68049]	
	25858.50	(0.20)	6(1, 5) - 6(0, 6)	EA	[68049]	
	25862.39	(0.20)	6(1, 5) - 6(0, 6)	AE	[68049]	
	25932.77	(0.20)	6(1, 5) - 6(0, 6)	EE	[68049]	
	26005.44	(0.20)	6(1, 5) - 6(0, 6)	AA	[68049]	
	27582.30	(0.20)	4(0, 4) - 3(1, 3)	AE	[68049]	
	27600.71	(0.20)	4(0, 4) - 3(1, 3)	EE	[68049]	
	27602.95	(0.20)	4(0, 4) - 3(1, 3)	AA	[68049]	
	28266.51	(0.20)	2(1, 2) - 1(0, 1)	EA	[68049]	
	28312.13	(0.20)	2(1, 2) - 1(0, 1)	AE	[68049]	
	28319.44	(0.20)	2(1, 2) - 1(0, 1)	EE	[68049]	
	28349.99	(0.20)	2(1, 2) - 1(0, 1)	AA	[68049]	
	28597.98	(0.20)	6(2, 4) - 6(1, 5)	AE	[68049]	
	28653.75	(0.20)	6(2, 4) - 6(1, 5)	EE	[68049]	
	28666.47	(0.20)	6(2, 4) - 6(1, 5)	AA	[68049]	
	28682.92	(0.20)	6(2, 4) - 6(1, 5)	EA	[68049]	
	28759.36	(0.20)	7(2, 5) - 7(1, 6)	AE	[68049]	
	28791.23	(0.20)	7(2, 5) - 7(1, 6)	EA	[68049]	
	28803.35	(0.20)	7(2, 5) - 7(1, 6)	EE	[68049]	
	28831.34	(0.20)	7(2, 5) - 7(1, 6)	AA	[68049]	
	29181.21	(0.20)	5(2, 3) - 5(1, 4)	AE	[68049]	
	29254.17	(0.20)	5(2, 3) - 5(1, 4)	AA	[68049]	
	29266.37	(0.20)	5(2, 3) - 5(1, 4)	EE	[68049]	
	29865.88	(0.20)	8(2, 6) - 8(1, 7)	AE	[68049]	
	29869.14	(0.20)	8(2, 6) - 8(1, 7)	EA	[68049]	
	29910.23	(0.20)	8(2, 6) - 8(1, 7)	EE	[68049]	
	29952.96	(0.20)	8(2, 6) - 8(1, 7)	AA	[68049]	
	30342.23	(0.20)	4(2, 2) - 4(1, 3)	AA	[68049]	
	30411.56	(0.20)	4(2, 2) - 4(1, 3)	EE	[68049]	
	31629.61	(0.20)	7(1, 6) - 7(0, 7)	AE	[68049]	
	31634.78	(0.20)	7(1, 6) - 7(0, 7)	EA	[68049]	
	31648.00	(0.20)	3(2, 1) - 3(1, 2)	AA	[68049]	
	31728.18	(0.20)	7(1, 6) - 7(0, 7)	EE	[68049]	
	31814.98	(0.20)	3(2, 1) - 3(1, 2)	EE	[68049]	
	31829.11	(0.20)	7(1, 6) - 7(0, 7)	AA	[68049]	
	32063.74	(0.20)	9(2, 7) - 9(1, 8)	EA	[68049]	
	32074.22	(0.20)	9(2, 7) - 9(1, 8)	AE	[68049]	
	32130.20	(0.20)	9(2, 7) - 9(1, 8)	EE	[68049]	
	32191.72	(0.20)	9(2, 7) - 9(1, 8)	AA	[68049]	
	32896.24	(0.20)	2(2, 0) - 2(1, 1)	AA	[68049]	
	33185.83	(0.20)	2(2, 0) - 2(1, 1)	EE	[68049]	
	35488.26	(0.20)	10(2, 8) - 10(1, 9)	EA	[68049]	
	35502.09	(0.20)	10(2, 8) - 10(1, 9)	AE	[68049]	
	35580.12	(0.20)	10(2, 8) - 10(1, 9)	EE	[68049]	
	35665.47	(0.20)	10(2, 8) - 10(1, 9)	AA	[68049]	
	35970.58	(0.20)	3(1, 3) - 2(0, 2)	EA	[68049]	
	35994.96	(0.20)	3(1, 3) - 2(0, 2)	AE	[68049]	
	36004.04	(0.20)	3(1, 3) - 2(0, 2)	EE	[68049]	
	36026.46	(0.20)	3(1, 3) - 2(0, 2)	AA	[68049]	
	37711.74	(0.20)	5(0, 5) - 4(1, 4)	EE	[68049]	
	37720.95	(0.20)	5(0, 5) - 4(1, 4)	AA	[68049]	
	38364.38	(0.20)	8(1, 7) - 8(0, 8)	AE	[68049]	
	38493.01	(0.20)	8(1, 7) - 8(0, 8)	EE	[68049]	
	sym-CH ₂ DCHCHCH ₃	26149.00	(0.20)	6(2, 4) - 6(1, 5)	E	[70067]
		26162.34	(0.20)	6(2, 4) - 6(1, 5)	A ₁	[70067]
		26710.08	(0.20)	7(2, 5) - 7(1, 6)	E	[70067]
		26737.00	(0.20)	7(2, 5) - 7(1, 6)	A ₁	[70067]
		28355.88	(0.20)	8(2, 6) - 8(1, 7)	E	[70067]
		28398.54	(0.20)	8(2, 6) - 8(1, 7)	A ₁	[70067]
		31237.86	(0.20)	9(2, 7) - 9(1, 8)	E	[70067]
31301.40		(0.20)	9(2, 7) - 9(1, 8)	A ₁	[70067]	

TABLE 27.5. Microwave spectrum of cis-2-butene — Continued

C₄H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Sym.	Ref.
asy-CH ₂ DCHCHCH ₃	28010.06	(0.20)	7(2, 5) - 7(1, 6)	E	[70067]
	28030.08	(0.20)	7(2, 5) - 7(1, 6)	A ₂	[70067]
	28031.04	(0.20)	7(2, 5) - 7(1, 6)	E	[70067]
	28051.38	(0.20)	7(2, 5) - 7(1, 6)	A ₁	[70067]
	28118.60	(0.20)	6(2, 4) - 6(1, 5)	E	[70067]
	28124.20	(0.20)	6(2, 4) - 6(1, 5)	A ₂	[70067]
	28138.72	(0.20)	6(2, 4) - 6(1, 5)	E	[70067]
	28145.26	(0.20)	6(2, 4) - 6(1, 5)	A ₁	[70067]
	28695.36	(0.20)	8(2, 6) - 8(1, 7)	E	[70067]
	28718.68	(0.20)	8(2, 6) - 8(1, 7)	E	[70067]
	28728.14	(0.20)	8(2, 6) - 8(1, 7)	A ₂	[70067]
	28751.68	(0.20)	8(2, 6) - 8(1, 7)	A ₁	[70067]
	30318.50	(0.20)	9(2, 7) - 9(1, 8)	E	[70067]
	30346.10	(0.20)	9(2, 7) - 9(1, 8)	E	[70067]
	30366.92	(0.20)	9(2, 7) - 9(1, 8)	A ₂	[70067]
	30394.52	(0.20)	9(2, 7) - 9(1, 8)	A ₁	[70067]
	32993.72	(0.20)	10(2, 8) - 10(1, 9)	E	[70067]
	33026.84	(0.20)	10(2, 8) - 10(1, 9)	E	[70067]
	33061.90	(0.20)	10(2, 8) - 10(1, 9)	A ₂	[70067]
	33095.24	(0.20)	10(2, 8) - 10(1, 9)	A ₁	[70067]
c-CH ₃ CDCHCH ₃	25894.22	(0.20)	6(2, 4) - 6(1, 5)	E ₁	[70067]
	25898.28	(0.20)	6(2, 4) - 6(1, 5)	E ₂	[70067]
	25911.20	(0.20)	6(2, 4) - 6(1, 5)	A ₁	[70067]
	26184.52	(0.20)	5(2, 3) - 5(1, 4)	A ₁	[70067]
	26185.86	(0.20)	5(2, 3) - 5(1, 4)	E ₁	[70067]
	26187.28	(0.20)	5(2, 3) - 5(1, 4)	E ₂	[70067]
	26476.60	(0.20)	7(2, 5) - 7(1, 6)	E ₄	[70067]
	26489.14	(0.20)	7(2, 5) - 7(1, 6)	E ₃	[70067]
	26513.04	(0.20)	7(2, 5) - 7(1, 6)	E ₂	[70067]
	26508.78	(0.20)	7(2, 5) - 7(1, 6)	E ₁	[70067]
	26539.20	(0.20)	7(2, 5) - 7(1, 6)	A ₁	[70067]
	28182.36	(0.20)	8(2, 6) - 8(1, 7)	E ₃	[70067]
	28187.60	(0.20)	8(2, 6) - 8(1, 7)	E ₄	[70067]
	28225.90	(0.20)	8(2, 6) - 8(1, 7)	E ₁	[70067]
	28229.18	(0.20)	8(2, 6) - 8(1, 7)	E ₂	[70067]
	28270.52	(0.20)	8(2, 6) - 8(1, 7)	A ₁	[70067]
	31129.54	(0.20)	9(2, 7) - 9(1, 8)	E ₃	[70067]
	31140.68	(0.20)	9(2, 7) - 9(1, 8)	E ₄	[70067]
	31196.14	(0.20)	9(2, 7) - 9(1, 8)	E ₁	[70067]
	31197.76	(0.20)	9(2, 7) - 9(1, 8)	E ₂	[70067]
31259.06	(0.20)	9(2, 7) - 9(1, 8)	A ₁	[70067]	
c-CH ₃ CDCHCH ₃	23584.76	(0.20)	5(2, 3) - 5(1, 4)	AE	[70067]
	23626.24	(0.20)	5(2, 3) - 5(1, 4)	EE	[70067]
	23629.56	(0.20)	5(2, 3) - 5(1, 4)	AA	[70067]
	23653.98	(0.20)	6(2, 4) - 6(1, 5)	AE	[70067]
	23659.86	(0.20)	5(2, 3) - 5(1, 4)	EA	[70067]
	23679.92	(0.20)	6(2, 4) - 5(1, 5)	EA	[70067]
	23683.20	(0.20)	6(2, 4) - 5(1, 5)	EE	[70067]
	23699.60	(0.20)	6(2, 4) - 5(1, 5)	AA	[70067]
	24754.92	(0.20)	7(2, 5) - 7(1, 6)	AE	[70067]
	24756.76	(0.20)	7(2, 5) - 7(1, 6)	EA	[70067]
	24783.72	(0.20)	7(2, 5) - 7(1, 6)	EE	[70067]
	24811.86	(0.20)	7(2, 5) - 7(1, 6)	AA	[70067]
	27076.08	(0.20)	8(2, 6) - 8(1, 7)	EA	[70067]
	27084.30	(0.20)	8(2, 6) - 8(1, 7)	AE	[70067]
	27123.02	(0.20)	8(2, 6) - 8(1, 7)	EE	[70067]
	27166.12	(0.20)	8(2, 6) - 8(1, 7)	AA	[70067]
	30769.50	(0.20)	9(2, 7) - 9(1, 8)	EA	[70067]
	30778.20	(0.20)	9(2, 7) - 9(1, 8)	AE	[70067]
	30836.28	(0.20)	9(2, 7) - 9(1, 8)	EE	[70067]
	30899.04	(0.20)	9(2, 7) - 9(1, 8)	AA	[70067]
c-CD ₃ CHCHCD ₃	18977.98	(0.02)	6(1, 5) - 6(0, 6)	EA + AE	[79039]
	18982.75	(0.02)	6(1, 5) - 6(0, 6)	EE	[79039]
	18987.52	(0.02)	6(1, 5) - 6(0, 6)	AA	[79039]
	22425.82	(0.02)	7(2, 5) - 7(1, 6)	EA + AE	[79039]
	22428.39	(0.02)	7(2, 5) - 7(1, 6)	EE	[79039]
	22430.96	(0.02)	7(2, 5) - 7(1, 6)	AA	[79039]

TABLE 27.5. Microwave spectrum of cis-2-butene — Continued

C₄H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Sym.	Ref.
	22523.63	(0.02)	6(2, 4) - 6(1, 5)	EA + AE	[79039]
	22525.90	(0.02)	6(2, 4) - 6(1, 5)	EE	[79039]
	22528.17	(0.02)	6(2, 4) - 6(1, 5)	AA	[79039]
	22948.10	(0.02)	8(2, 6) - 8(1, 7)	EA + AE	[79039]
	22951.22	(0.02)	8(2, 6) - 8(1, 7)	EE	[79039]
	22954.28	(0.02)	8(2, 6) - 8(1, 7)	AA	[79039]
	26300.16	(0.02)	10(2, 8) - 10(1, 9)	EA + AE	[79039]
	26305.34	(0.02)	10(2, 8) - 10(1, 9)	EE	[79039]
	26310.50	(0.02)	10(2, 8) - 10(1, 9)	AA	[79039]
	30480.30	(0.02)	5(0, 5) - 4(1, 4)	EA + AE	[79039]
	30480.95	(0.02)	5(0, 5) - 4(1, 4)	EE	[79039]
	30481.595	(0.020)	5(0, 5) - 4(1, 4)	AA	[79039]
	34038.54	(0.02)	13(3, 10) - 13(2, 11)	AA	[79039]
	34041.24	(0.02)	13(3, 10) - 13(2, 11)	EE	[79039]
	34043.84	(0.02)	13(3, 10) - 13(2, 11)	AA	[79039]
	34662.04	(0.02)	14(3, 11) - 14(2, 12)	EA + AE	[79039]
	34665.68	(0.02)	14(3, 11) - 14(2, 12)	EE	[79039]
	34669.38	(0.02)	14(3, 11) - 14(2, 12)	AA	[79039]
	35110.25	(0.02)	4(1, 4) - 3(0, 3)	EA + AE	[79039]
	35111.255	(0.020)	4(1, 4) - 3(0, 3)	EE	[79039]
	35112.20	(0.02)	4(1, 4) - 3(0, 3)	AA	[79039]
	38508.14	(0.02)	6(0, 6) - 5(1, 5)	EA + AE	[79039]
	38509.02	(0.02)	6(0, 6) - 5(1, 5)	EE	[79039]
	38510.00	(0.02)	6(0, 6) - 5(1, 5)	AA	[79039]
c-CD ₃ CDCDCD ₃	18842.08	(0.02)	6(2, 4) - 6(1, 5)	EA + AE	[79039]
	18843.72	(0.02)	6(2, 4) - 6(1, 5)	EE	[79039]
	18845.36	(0.02)	6(2, 4) - 6(1, 5)	AA	[79039]
	18998.52	(0.02)	5(2, 3) - 5(1, 4)	EA + AE	[79039]
	18999.95	(0.02)	5(2, 3) - 5(1, 4)	EE	[79039]
	19001.39	(0.02)	5(2, 3) - 5(1, 4)	AA	[79039]
	19371.04	(0.02)	7(2, 5) - 7(1, 6)	EA + AE	[79039]
	19373.13	(0.02)	7(2, 5) - 7(1, 6)	EE	[79039]
	19375.19	(0.02)	7(2, 5) - 7(1, 6)	AA	[79039]
	23049.56	(0.02)	9(2, 7) - 9(1, 8)	EA + AE	[79039]
	23053.28	(0.02)	9(2, 7) - 9(1, 8)	EE	[79039]
	23056.96	(0.02)	9(2, 7) - 9(1, 8)	AA	[79039]
	30364.50	(0.02)	5(0, 5) - 4(1, 4)	EE	[79039]
	30450.23	(0.02)	13(3, 10) - 13(2, 11)	EA + AE	[79039]
	30453.78	(0.02)	13(3, 10) - 13(2, 11)	EE	[79039]
	30457.31	(0.02)	13(3, 10) - 13(2, 11)	AA	[79039]
	32261.00	(0.02)	4(1, 4) - 3(0, 3)	EE	[79039]
	33039.96	(0.02)	14(3, 11) - 14(2, 12)	EA + AE	[79039]
	33044.76	(0.02)	14(3, 11) - 14(2, 12)	EE	[79039]
	33049.58	(0.02)	14(3, 11) - 14(2, 12)	AA	[79039]
	37752.00	(0.02)	16(4, 12) - 16(3, 13)	EA + AE	[79039]
	37753.20	(0.02)	16(4, 12) - 16(3, 13)	EE	[79039]
	37754.46	(0.02)	16(4, 12) - 16(3, 13)	AA	[79039]
	37870.00	(0.02)	6(0, 6) - 5(1, 5)	EE	[79039]

Table 28.1. Molecular constants for isobutylene (2-methyl propene) in the ground and torsionally excited states.

Parameter	Ground State	(CH ₃) ₂ C=CH ₂	
		v _t = 1 ₁ State	v _t = 1 ₂ State
<u>Rotational constants^a [75058]</u>			
A (MHz)	9133.31(3)	9132.01(3)	9140.61(3)
B (MHz)	8381.80(3)	8369.09(3)	8353.22(3)
C (MHz)	4615.97(2)	4613.46(2)	4613.41(2)
Δ _{JK} (kHz)	-16.70(7)		
Δ _J (kHz)	7.88(46)		
δ _J (Hz)	-65.3(30)		
δ _K (kHz)	-19.385(48)		
<u>Internal Rotation Constants [75058]</u>			
I _α (u Å ²)	3.18(1)		3.18 ^b
θ	58.21(6) ^o		58.21 ^b
V ₃ (cm ⁻¹)	759.8(32)		767.9(35)
V ₁₂ ⁱ (cm ⁻¹)			-74.(11)
Δ ₀ (MHz)	-9.659(58)		
ρ	0.05620(20)		
β (rad)	0.5172(12)		
<u>Electric Dipole Moment [61014]</u>			
μ _b (D)	0.503(9)		

^aRepresentation III^r was used for AA state.^bValues fixed.

Table 28.2. Rotational analysis of isobutylene AA state from the present study.

Parameter	AA State
A'' (MHz)	9133.392(35)
B'' (MHz)	8381.846(35)
C'' (MHz)	4615.966(35)
τ ₁ (MHz)	-0.021(25)
τ ₂ (MHz)	-0.0054(84)
τ ₃ ^a (MHz)	0.60(25)
τ _{aaaa} (MHz)	-0.028(8)
τ _{bbbb} (MHz)	-0.029(8)
τ _{cccc} (MHz)	0.0041(85)

^aThe value of τ₃ is fixed by setting R₆ = 0.Table 28.3. Rotational constants for deuterated and ¹³C isotopic species of isobutylene.

Species	A (MHz)	B (MHz)	C (MHz)	Reference
s-CH ₂ DCH ₃ CCH ₂	9132.59	7788.98	4431.05	[61014]
a-CH ₂ DCH ₃ CCH ₂	8819.46	7981.08	4469.59	[61014]
(CH ₃) ₂ CCHD	8693.49	8114.67	4422.67	[63027]
(CH ₃) ₂ C ¹³ CH ₂	8810.08	8381.73	4531.84	[63027]
CH ₃ ¹³ CH ₃ CCH ₂	9074.31	8149.00	4529.72	[63027]

TABLE 28.4. Microwave spectrum of isobutylene — Continued

C₄H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$	$- J''(K_{-1}, K_{+1})$	$\nu_1 \nu_2$	Sym.	Vib. state	Ref.
	22128.05	(0.10)	2(0, 2)	- 1(1, 1)				[61014]
	22320.86	(0.10)	6(5, 2)	- 6(4, 3)				[61014]
	22976.59	(0.10)	10(7, 3)	- 10(6, 4)				[61014]
	22981.28	(0.10)	2(1, 2)	- 1(0, 1)				[61014]
	23490.64	(0.10)	7(6, 2)	- 7(5, 3)				[61014]
	23524.30	(0.10)	7(7, 1)	- 7(6, 2)		AE + EA		[61014]
	23524.94	(0.10)	7(7, 1)	- 7(6, 2)		EE		[61014]
	23525.58	(0.10)	7(7, 1)	- 7(6, 2)		AA		[61014]
	23993.911	(0.030)	8(8, 0)	- 8(7, 1)		AE		[75058]
	23994.287	(0.030)	8(8, 0)	- 8(7, 1)		EA		[75058]
	23994.821	(0.030)	8(8, 0)	- 8(7, 1)		EE		[75058]
	23995.551	(0.030)	8(8, 0)	- 8(7, 1)		AA		[75058]
	24638.80	(0.10)	9(6, 3)	- 9(5, 4)				[61014]
	26574.382	(0.030)	8(8, 1)	- 8(7, 2)		EA		[75058]
	26574.774	(0.030)	8(8, 1)	- 8(7, 2)		AE		[75058]
	26575.365	(0.030)	8(8, 1)	- 8(7, 2)		EE		[75058]
	26576.146	(0.030)	8(8, 1)	- 8(7, 2)		AA		[75058]
	28121.48	(0.10)	6(3, 3)	- 6(2, 4)				[61014]
	28219.237	(0.030)	9(9, 0)	- 9(8, 1)		AE		[75058]
	28220.382	(0.030)	9(9, 0)	- 9(8, 1)		EE		[75058]
	28221.066	(0.030)	9(9, 0)	- 9(8, 1)		AA		[75058]
	28330.145	(0.030)	9(9, 0)	- 9(8, 1)		EA		[75058]
	28557.285	(0.10)	5(2, 3)	- 5(1, 4)				[61014]
	28759.698	(0.10)	4(2, 3)	- 4(1, 4)		A ₂ A ₁	1ν ₂	[75058]
	28765.930	(0.10)	4(2, 3)	- 4(1, 4)		EE	1ν ₂	[75058]
	28771.06	(0.10)	4(1, 3)	- 4(0, 4)				[61014]
	28772.171	(0.10)	4(1, 3)	- 4(0, 4)	A ₂	E + EA ₁	1ν ₂	[75058]
	28775.67	(0.10)	6(4, 3)	- 6(3, 4)				[61014]
	28794.628	(0.030)	4(2, 3)	- 4(1, 4)		A ₁ A ₂	1ν ₁	[75058]
	28799.251	(0.030)	4(2, 3)	- 4(1, 4)		EE	1ν ₁	[75058]
	28803.859	(0.030)	4(2, 3)	- 4(1, 4)	A ₁	E + EA ₂	1ν ₁	[75058]
	28830.61	(0.10)	4(2, 3)	- 4(1, 4)				[61014]
	28851.31	(0.10)	7(5, 3)	- 7(4, 4)				[61014]
	29089.07	(0.10)	8(6, 3)	- 8(5, 4)				[61014]
	29851.100	(0.030)	9(9, 1)	- 9(8, 2)		EA		[75058]
	29852.000	(0.030)	9(9, 1)	- 9(8, 2)		AE		[75058]
	29852.580	(0.030)	9(9, 1)	- 9(8, 2)		EE		[75058]
	29853.583	(0.030)	9(9, 1)	- 9(8, 2)		AA		[75058]
	29908.76	(0.10)	14(12, 2)	- 14(11, 3)		AE + EA		[61014]
	29909.89	(0.10)	14(12, 2)	- 14(11, 3)		EE		[61014]
	29910.98	(0.10)	14(12, 2)	- 14(11, 3)		AA		[61014]
	31768.96	(0.10)	3(0, 3)	- 2(1, 2)				[61014]
	31879.31	(0.10)	3(1, 3)	- 2(0, 2)				[61014]
	31932.784	(0.030)	12(11, 1)	- 12(10, 2)		AE		[75058]
	31933.042	(0.030)	12(11, 1)	- 12(10, 2)		EA		[75058]
	31933.956	(0.030)	12(11, 1)	- 12(10, 2)		EE		[75058]
	31934.994	(0.030)	12(11, 1)	- 12(10, 2)		AA		[75058]
	31937.872	(0.030)	17(14, 3)	- 17(13, 4)		AE + EA		[75058]
	31938.959	(0.030)	17(14, 3)	- 17(13, 4)		EE		[75058]
	31940.047	(0.030)	17(14, 3)	- 17(13, 4)		AA		[75058]
	32015.95	(0.10)	2(2, 1)	- 1(1, 0)				[61014]
	33291.123	(0.030)	10(10, 1)	- 10(9, 2)		EA		[75058]
	33293.126	(0.030)	10(10, 1)	- 10(9, 2)		AE		[75058]
	33293.497	(0.030)	10(10, 1)	- 10(9, 2)		EE		[75058]
	33294.910	(0.030)	10(10, 1)	- 10(9, 2)		AA		[75058]
<i>sym</i> -CH ₂ DCH ₃ CCH ₂	18852.70	(0.10)	3(1, 2)	- 3(0, 3)				[61014]
	20334.26	(0.10)	3(2, 2)	- 3(1, 3)				[61014]
	20752.87	(0.10)	2(0, 2)	- 1(1, 1)				[61014]
	22425.74	(0.10)	2(1, 2)	- 1(0, 1)				[61014]
	30377.99	(0.10)	3(0, 3)	- 2(1, 2)				[61014]
	30759.55	(0.10)	3(1, 3)	- 2(0, 2)				[61014]
	31828.82	(0.10)	2(2, 1)	- 1(1, 0)				[61014]
<i>asy</i> -CH ₂ DCH ₃ CCH ₂	18347.00	(0.10)	4(2, 2)	- 4(1, 3)				[61014]
	19730.99	(0.10)	3(2, 2)	- 3(1, 3)				[61014]
	20065.05	(0.10)	4(3, 2)	- 4(2, 3)				[61014]
	21256.85	(0.10)	2(0, 1)	- 1(1, 1)				[61014]
	22228.22	(0.10)	2(1, 2)	- 1(0, 1)				[61014]

TABLE 28.4. Microwave spectrum of isobutylene

C₄H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	$\nu_1 \nu_2$	Sym.	Vib. state	Ref.
(CH ₃) ₂ CCH ₂	9016.803	(0.030)	4(4, 0) - 4(3, 1)		AE + EA		[75058]
	9017.080	(0.030)	4(4, 0) - 4(3, 1)		EE		[75058]
	9017.356	(0.030)	4(4, 0) - 4(3, 1)		AA		[75058]
	10658.393	(0.030)	3(2, 1) - 3(1, 2)		A ₂ A ₁	1ν ₂	[75058]
	10659.734	(0.030)	3(2, 1) - 3(1, 2)		EE	1ν ₂	[75058]
	10660.932	(0.030)	3(2, 1) - 3(1, 2)		A ₂ E	1ν ₂	[75058]
	10661.227	(0.030)	3(2, 1) - 3(1, 2)		EA ₁	1ν ₂	[75058]
	10704.889	(0.030)	3(2, 1) - 3(1, 2)		A ₁ A ₂	1ν ₁	[75058]
	10705.844	(0.030)	3(2, 1) - 3(1, 2)		EE	1ν ₁	[75058]
	10706.846	(0.030)	3(2, 1) - 3(1, 2)	A ₁	E + EA ₂	1ν ₁	[75058]
	11331.276	(0.030)	2(1, 1) - 2(0, 2)		A ₂ A ₁	1ν ₂	[75058]
	11332.948	(0.030)	2(1, 1) - 2(0, 2)		EE	1ν ₂	[75058]
	11334.640	(0.030)	2(1, 1) - 2(0, 2)	A ₂	E + EA ₁	1ν ₂	[75058]
	11371.830	(0.030)	2(1, 1) - 2(0, 2)		A ₁ A ₂	1ν ₁	[75058]
	11373.090	(0.030)	2(1, 1) - 2(0, 2)		EE	1ν ₁	[75058]
	11374.192	(0.030)	2(1, 1) - 2(0, 2)	A ₁	E + EA ₂	1ν ₁	[75058]
	11994.512	(0.030)	5 5, 0) - 5(4, 1)		AE + EA		[75058]
	11994.926	(0.030)	5 5, 0) - 5(4, 1)		EE		[75058]
	11995.316	(0.030)	5 5, 0) - 5(4, 1)		AA		[75058]
	12771.162	(0.030)	7(6, 1) - 7(5, 2)		AE + EA		[75058]
	12771.509	(0.030)	7(6, 1) - 7(5, 2)		EE		[75058]
	12771.852	(0.030)	7(6, 1) - 7(5, 2)		AA		[75058]
	13555.767	(0.030)	2(2, 1) - 2(1, 2)		A ₁ A ₂	1ν ₁	[75058]
	13558.812	(0.030)	2(2, 1) - 2(1, 2)		EE	1ν ₁	[75058]
	13561.588	(0.030)	2(2, 1) - 2(1, 2)		EA ₂	1ν ₁	[75058]
	13562.053	(0.030)	2(2, 1) - 2(1, 2)		A ₁ E	1ν ₁	[75058]
	13581.727	(0.030)	2(2, 1) - 2(1, 2)		A ₁ A ₂	1ν ₂	[75058]
	13585.767	(0.030)	2(2, 1) - 2(1, 2)		EE	1ν ₂	[75058]
	13589.411	(0.030)	2(2, 1) - 2(1, 2)		EA ₁	1ν ₂	[75058]
	13590.397	(0.030)	2(2, 1) - 2(1, 2)		A ₂ E	1ν ₂	[75058]
	13745.462	(0.030)	1(1, 1) - 0(0, 0)		A ₁ A ₂	1ν ₁	[75058]
	13746.535	(0.030)	1(1, 1) - 0(0, 0)		EE	1ν ₁	[75058]
	13747.575	(0.030)	1(1, 1) - 0(0, 0)	A ₁	E + EA ₂	1ν ₁	[75058]
	13754.019	(0.030)	1(1, 1) - 0(0, 0)		A ₂ A ₁	1ν ₂	[75058]
	13755.377	(0.030)	1(1, 1) - 0(0, 0)		EE	1ν ₂	[75058]
	13756.602	(0.030)	1(1, 1) - 0(0, 0)		EA ₁	1ν ₂	[75058]
	15320.412	(0.030)	8(7, 1) - 8(6, 2)		AE + EA		[75058]
	15320.930	(0.030)	8(7, 1) - 8(6, 2)		EE		[75058]
	15321.466	(0.030)	8(7, 1) - 8(6, 2)		AA		[75058]
	15646.492	(0.030)	6(6, 0) - 6(5, 1)		AE + EA		[75058]
	15647.046	(0.030)	6(6, 0) - 6(5, 1)		EE		[75058]
	15647.607	(0.030)	6(6, 0) - 6(5, 1)		AA		[75058]
	18358.45	(0.10)	5 5, 1) - 5(4, 2)				[61014]
	18473.09	(0.10)	11(9, 2) - 11(8, 3)		EE		[61014]
	18473.73	(0.10)	11(9, 2) - 11(8, 3)		AA		[61014]
	18703.70	(0.10)	5 3, 2) - 5(2, 3)				[61014]
	18746.62	(0.10)	9 8, 1) - 9(7, 2)		AE + EA		[61014]
	18747.34	(0.10)	9 8, 1) - 9(7, 2)		EE		[61014]
	18748.06	(0.10)	9 8, 1) - 9(7, 2)		EE		[61014]
	18748.06	(0.10)	9 8, 1) - 9(7, 2)		AA		[61014]
	19669.25	(0.10)	4(2, 2) - 4(1, 3)				[61014]
	19736.00	(0.10)	7(7, 0) - 7(6, 1)		AE + EA		[61014]
	19736.70	(0.10)	7(7, 0) - 7(6, 1)		EE		[61014]
	20202.223	(0.030)	3(1, 2) - 3(0, 3)		EE	1ν ₂	[75058]
	20198.505	(0.030)	3(1, 2) - 3(0, 3)		A ₂ A ₁	1ν ₂	[75058]
	20205.970	(0.030)	3(1, 2) - 3(0, 3)	A ₂	E + EA ₁	1ν ₂	[75058]
	20244.318	(0.030)	3(1, 2) - 3(0, 3)		A ₂ A ₁	1ν ₁	[75058]
	20247.070	(0.030)	3(1, 2) - 3(0, 3)		EE	1ν ₁	[75058]
	20249.838	(0.030)	3(1, 2) - 3(0, 3)	A ₁	E + EA ₂	1ν ₁	[75058]
	20279.79	(0.10)	3(1, 2) - 3(0, 3)				[61014]
	20765.21	(0.10)	6(6, 1) - 6(5, 2)		AE + EA		[61014]
	20766.70	(0.10)	6(6, 1) - 6(5, 2)		EE		[61014]
	20767.23	(0.10)	6(6, 1) - 6(5, 2)		AA		[61014]
	20767.71	(0.10)	3(2, 2) - 3(1, 3)				[61014]
	21026.60	(0.10)	4(3, 2) - 4(2, 3)				[61014]
	21448.58	(0.10)	12(10, 2) - 12(9, 3)		AE + EA		[61014]
	21449.36	(0.10)	12(10, 2) - 12(9, 3)		EE		[61014]
	21450.11	(0.10)	12(10, 2) - 12(9, 3)		AA		[61014]
	21519.40	(0.10)	5 4, 2) - 5 3, 3)				[61014]

TABLE 28.4. Microwave spectrum of isobutylene — Continued

C₄H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	$\nu_1 \nu_2$	Sym.	Vib. state	Ref.
(CH ₃) ₂ CCDH	30657.22	(0.10)	3(0, 3)	- 2(1, 2)			[61014]
	30803.61	(0.10)	3(1, 3)	- 2(0, 2)			[61014]
	30927.96	(0.10)	2(2, 1)	- 1(1, 0)			[61014]
	19944.54	(0.10)	3(1, 2)	- 3(1, 3)			[63027]
	19639.41	(0.10)	3(1, 2)	- 3(0, 3)			[63027]
	21319.80	(0.10)	2(0, 2)	- 1(1, 1)			[63027]
	21961.51	(0.10)	2(1, 2)	- 1(0, 1)			[63027]
	30475.68	(0.10)	3(0, 3)	- 2(1, 2)			[63027]
	30503.15	(0.10)	2(2, 1)	- 1(1, 0)			[63027]
	30542.80	(0.10)	3(1, 3)	- 2(0, 2)			[63027]
¹³ CH ₃ (CH ₃)CCH ₂	13604.08	(0.10)	1(1, 1)	- 0(0, 0)			[63027]
	18905.09	(0.10)	4(2, 2)	- 4(1, 3)			[63027]
	19764.88	(0.10)	3(1, 2)	- 3(0, 3)			[63027]
	20889.82	(0.10)	4(3, 2)	- 4(2, 3)			[63027]
	21582.34	(0.10)	2(0, 2)	- 1(1, 1)			[63027]
	22663.50	(0.10)	2(1, 2)	- 1(0, 1)			[63027]
	31153.16	(0.10)	3(0, 3)	- 2(1, 2)			[63027]
	31325.69	(0.10)	3(1, 3)	- 2(0, 2)			[63027]
	31752.65	(0.10)	2(2, 1)	- 1(1, 0)			[63027]
	13342.01	(0.10)	1(1, 1)	- 0(0, 0)			[63027]
(CH ₃) ₂ C ¹³ CH ₂	19947.74	(0.10)	4(2, 2)	- 4(1, 3)			[63027]
	20174.97	(0.10)	3(1, 2)	- 3(0, 3)			[63027]
	20340.93	(0.10)	3(2, 2)	- 3(1, 3)			[63027]
	20429.62	(0.10)	4(3, 2)	- 4(2, 3)			[63027]
	21943.47	(0.10)	2(0, 2)	- 1(1, 1)			[63027]
	22405.60	(0.10)	2(1, 2)	- 1(0, 1)			[63027]
	30962.08	(0.10)	2(2, 1)	- 1(1, 0)			[63027]
	31233.01	(0.10)	3(0, 3)	- 2(1, 2)			[63027]
	31268.52	(0.10)	3(1, 3)	- 2(0, 2)			[63027]

Table 29.1. Molecular constants for methylcyclopropane.

Parameter	CH ₃ CHCH ₂ CH ₂
<u>Rotational Constants</u>	
A'' (MHz)	15503.225(33)
B'' (MHz)	6363.4072(78)
C'' (MHz)	5586.4839(69)
τ ₁ (MHz)	-0.0077(53)
τ ₂ (MHz)	-0.0017(15)
τ ₃ ^a (MHz)	0.147(58)
τ _{aaaa} (MHz)	-0.112(41)
τ _{bbbb} (MHz)	-0.0028(6)
<u>Internal Rotation Barrier</u> [68048]	
V ₃ (cm ⁻¹)	1001.(18)
<u>Dipole Moments</u> [68048]	
μ _a (D)	0.097(1)
μ _c (D)	0.100(5)

^aThe value of τ₃ is fixed by setting R₆ = 0.

TABLE 29.2. Microwave spectrum of methylcyclopropane

C₄H₈

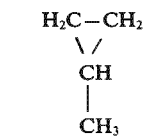
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	v_1	Sym.	Ref.
CH ₂ CH ₂ CHCH ₃	11949.95	(0.05)	1(0, 1) - 0(0, 0)	0		[68048]
	16017.18	(0.05)	8(2, 7) - 8(1, 7)	0		[68048]
	20867.76	(0.05)	6(2, 5) - 6(1, 5)	0		[68048]
	21157.80	(0.05)	21(4, 18) - 21(3, 18)	0	E	[68048]
	21158.03	(0.05)	21(4, 18) - 21(3, 18)	0	A	[68048]
	21868.57	(0.05)	1(1, 0) - 0(0, 0)	0		[68048]
	22979.60	(0.05)	5(2, 4) - 5(1, 4)	0		[68048]
	23122.90	(0.05)	2(1, 2) - 1(1, 1)	0		[68048]
	23550.83	(0.05)	27(5, 23) - 27(4, 23)	0	E	[68048]
	23551.11	(0.05)	27(5, 23) - 27(4, 23)	0	A	[68048]
	23852.38	(0.05)	2(0, 2) - 1(0, 1)	0		[68048]
	24676.68	(0.05)	2(1, 1) - 1(1, 0)	0		[68048]
	24800.03	(0.05)	4(2, 3) - 4(1, 3)	0		[68048]
	24917.95	(0.05)	3(0, 3) - 2(1, 1)	0		[68048]
	25230.80	(0.05)	30(6, 24) - 30(6, 25)	0	A	[68048]
	25231.12	(0.05)	30(6, 24) - 30(6, 25)	0	E	[68048]
	25399.07	(0.05)	13(3, 11) - 13(2, 11)	0		[68048]
	25780.06	(0.05)	20(4, 17) - 20(3, 17)	0	E	[68048]
	25780.30	(0.05)	20(4, 17) - 20(3, 17)	0	A	[68048]
	30656.08	(0.05)	19(4, 16) - 19(3, 16)	0	E	[68048]
	30656.36	(0.05)	19(4, 16) - 19(3, 16)	0	A	[68048]
	33257.28	(0.05)	4(2, 2) - 4(1, 4)	0		[68048]
	34595.38	(0.05)	2(1, 1) - 1(0, 1)	0		[68048]
	35660.95	(0.05)	3(0, 3) - 2(0, 2)	0		[68048]

Table 29.1A. Molecular constants for cyclobutane-d₁.

Parameter	Equatorial	Axial
A (MHz)	10617.908(17)	10377.613(18)
B (MHz)	9817.535(17)	9975.708(18)
C (MHz)	6050.794(17)	6193.449(18)
Δ_J (kHz)	4.3(22)	5.3(20)
Δ_{JK} (kHz)	-3.18(89)	-4.4(12)
Δ_K (kHz)	6.04(66)	6.25(83)
δ_J (kHz)	0.79(13)	0.95(19)
δ_K (kHz)	1.31(37)	0.65(45)
H_{KJ} (Hz)	-0.0079(6)	-0.014(7)
<u>Electric Dipole Moment</u> [87024]		
μ_a (D)	0.0043(14)	---
μ_c (D)	---	0.0043(14)

TABLE 29.2.a. Microwave spectrum of cyclobutane-*d*₁C₄H₈

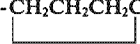
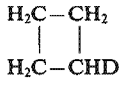
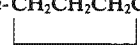
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.	
ϵ -CH ₂ CH ₂ CH ₂ CHD 	12739.495	(0.030)	21(16, 5) - 21(16, 6)	[87024]	
	12772.716	(0.030)	33(25, 8) - 33(25, 9)	[87024]	
	13012.180	(0.030)	29(22, 7) - 29(22, 8)	[87024]	
	13020.253	(0.030)	25(19, 6) - 25(19, 7)	[87024]	
	13145.023	(0.030)	20(15, 6) - 20(14, 6)	[87024]	
		13688.896	(0.030)	8(7, 2) - 8(6, 2)	[87024]
		13815.810	(0.030)	2(2, 1) - 2(0, 2)	[87024]
		14134.661	(0.030)	17(13, 5) - 17(12, 5)	[87024]
		14308.461	(0.030)	12(9, 3) - 12(9, 4)	[87024]
		14417.826	(0.030)	7(5, 2) - 7(5, 3)	[87024]
		14592.582	(0.030)	11(9, 3) - 11(8, 3)	[87024]
		14676.210	(0.030)	14(11, 4) - 14(10, 4)	[87024]
		15526.665	(0.030)	3(3, 1) - 3(1, 2)	[87024]
		15868.311	(0.030)	1(0, 1) - 0(0, 0)	[87024]
		15966.320	(0.030)	16(12, 4) - 16(12, 5)	[87024]
	α -CH ₂ CH ₂ CH ₂ CHD 	16593.370	(0.030)	6(4, 2) - 6(4, 3)	[87024]
		16851.363	(0.030)	40(30,10) - 40(30,11)	[87024]
		17064.296	(0.030)	20(15, 5) - 20(15, 6)	[87024]
		17320.902	(0.030)	24(18, 7) - 24(17, 7)	[87024]
		17447.226	(0.030)	36(27, 9) - 36(27,10)	[87024]
17618.221		(0.030)	11(8, 3) - 11(8, 4)	[87024]	
17692.049		(0.030)	24(18, 6) - 24(18, 7)	[87024]	
17822.241		(0.030)	32(24, 8) - 32(24, 9)	[87024]	
28655.670		(0.020)	2(0, 2) - 1(0, 1)	[87024]	
40070.4		(0.1)	2(1, 1) - 1(0, 1)	[87024]	
12582.760		(0.030)	2(2, 1) - 2(0, 2)	[87024]	
12582.760		(0.030)	11(10, 2) - 11(9, 2)	[87024]	
12873.781		(0.030)	19(16, 4) - 19(15, 4)	[87024]	
12878.909		(0.030)	23(19, 4) - 23(19, 5)	[87024]	
12880.044		(0.030)	17(14, 3) - 17(14, 4)	[87024]	
13127.925		(0.030)	15(13, 3) - 15(12, 3)	[87024]	
13324.220		(0.030)	3(3, 1) - 3(1, 2)	[87024]	
13455.845		(0.030)	10(8, 2) - 10(8, 3)	[87024]	
13713.366		(0.030)	34(28, 6) - 34(28, 7)	[87024]	
13845.385		(0.030)	8(8, 1) - 8(7, 1)	[87024]	
14392.214	(0.100)	28(23, 6) - 28(22, 6)	[87024]		
14454.588	(0.030)	4(4, 1) - 4(2, 2)	[87024]		
15028.504	(0.100)	28(23, 5) - 28(23, 6)	[87024]		
15037.261	(0.030)	9(7, 2) - 9(7, 3)	[87024]		
15198.348	(0.030)	16(13, 3) - 16(13, 4)	[87024]		
15244.820	(0.030)	39(32, 7) - 39(32, 8)	[87024]		
15619.761	(0.030)	22(18, 4) - 22(18, 5)	[87024]		
15656.575	(0.100)	24(20, 5) - 24(19, 5)	[87024]		
15757.851	(0.030)	12(11, 2) - 12(10, 2)	[87024]		
16071.080	(0.030)	5(5, 1) - 5(3, 2)	[87024]		
16169.136	(0.030)	1(0, 1) - 0(0, 0)	[87024]		
16436.670	(0.030)	8(6, 2) - 8(6, 3)	[87024]		
16440.175	(0.100)	20(17, 4) - 20(16, 4)	[87024]		
16543.855	(0.030)	16(14, 3) - 16(13, 3)	[87024]		
16888.486	(0.030)	9(9, 1) - 9(8, 1)	[87024]		
17054.099	(0.100)	33(27, 6) - 33(27, 7)	[87024]		
17478.178	(0.030)	15(12, 3) - 15(12, 4)	[87024]		
17608.137	(0.030)	7(5, 2) - 7(5, 3)	[87024]		
28927.6	(0.1)	2(0, 2) - 1(0, 1)	[87024]		
40304.550	(0.020)	2(1, 1) - 1(0, 1)	[87024]		

Table 30.1. Molecular constants for the isobutane species: $(\text{CH}_3)_3\text{CH}$, $(\text{CH}_3)_3^{13}\text{CH}$ and $(\text{CH}_3)_3\text{CD}$.

Parameter		$(\text{CH}_3)_3\text{CH}$	$(\text{CH}_3)_3^{13}\text{CH}$	$(\text{CH}_3)_3\text{CD}$
B_0	(MHz)	7789.45(3)	7773.88(3)	7540.82(2)
B_{τ_a}	(MHz)	7782.84(5)		
B_{τ_e}	(MHz)	7774.67(5)		
B_{δ_a}	(MHz)	7790.3(3)		
B_{δ_e}	(MHz)	7795.0(3)		
D_J	(MHz)	0.011(4)		
$q_l(\tau_e)$	(MHz)	21.0		
$q_l(\delta_e)$	(MHz)	17.		
μ	(D)	0.132(1)		0.141(2)
Reference		[58010]	[60010]	[60010]

Table 30.2. Rotational constants for asymmetric-rotor species of isobutane. [60010]

Parameter	$^{13}\text{CH}_3(\text{CH}_3)_2\text{CH}$	sym- $\text{CH}_2\text{D}(\text{CH}_3)_2\text{CH}$	asy- $\text{CH}_2\text{D}(\text{CH}_3)_2\text{CH}$
A (MHz)	7788.28(5)	7629.15(20)	7782.70(3)
B (MHz)	7546.10(5)	7378.95(40)	7259.37(3)
C (MHz)	4431.(45)	4466.(140)	4319.(7)

TABLE 30.3. Microwave spectrum of isobutane

 C_4H_{10}

Isotopic species	Frequency (MHz)	Unc (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
$(\text{CH}_3)_3\text{CH}$	15578.9	(0.10)	1() - 0()		[58010]
	31098.35	(0.10)	2() - 1()	$1\nu_t e$	[58010]
	31130.99	(0.10)	2() - 1()	$1\nu_t a$	[58010]
	31157.46	(0.10)	2() - 1()		[58010]
	31161.00	(0.10)	2() - 1()	$1\nu_d a$	[58010]
	31180.00	(0.10)	2() - 1()	$1\nu_d e$	[60010]
$(\text{CH}_3)_3^{13}\text{CH}$	31095.18	(0.10)	2() - 1()		[60010]
$(\text{CH}_3)_3\text{CD}$	31162.95	(0.05)	2() - 1()		[60010]
$^{13}\text{CH}_3(\text{CH}_3)_2\text{CH}$	30426.24	(0.10)	2(1, 1) - 1(0, 1)		[60010]
	30682.00	(0.10)	2(2, 0) - 1(1, 0)		[60010]
	30910.58	(0.10)	2(2, 1) - 1(1, 1)		[60010]
	29765.6	(0.1)	2(1, 1) - 1(0, 1)		[60010]
sym- $\text{CH}_2\text{D}(\text{CH}_3)_2\text{CH}$	30031.28	(0.10)	2(2, 0) - 1(1, 0)		[60010]
	30266.06	(0.20)	2(2, 1) - 1(1, 1)		[60010]
	29560.45	(0.05)	2(1, 1) - 1(0, 1)		[60010]
asy- $\text{CH}_2\text{D}(\text{CH}_3)_2\text{CH}$	30147.92	(0.05)	2(2, 0) - 1(1, 0)		[60010]
	30607.11	(0.05)	2(2, 1) - 1(1, 1)		[60010]

Table 31.1. Molecular constants for the C₅H radical. [86004]

Parameter	Value	
A _{eff}	(MHz)	710039.(33)
B	(MHz)	2395.131(1)
D	(MHz)	0.129(1)x10 ⁻³
p + 2q	(MHz)	3.72(7)
q	(MHz)	-0.304(2)
B _{eff} (² Π _{1/2})	(MHz)	2387.003(2)
B _{eff} (² Π _{3/2})	(MHz)	2403.241(6)
D _{eff} (² Π _{1/2})	(MHz)	0.041(1)x10 ⁻³
D _{eff} (² Π _{3/2})	(MHz)	0.211(2)x10 ⁻³
<u>Hyperfine parameters</u> [87012]		
a' = a - $\frac{(b+c)}{2}$	(MHz)	20.04(15)
d	(MHz)	10.9(6)

TABLE 31.2. Microwave spectrum of C₅H radicalC₅H

Isotopic species	Frequency (MHz)	Unc. (MHz)	J' - J''	P	F' - F''	Vib. state	Ref.
CCCCCH ² Π _{1/2}	21480.823	(0.022)	9/2 - 7/2	a	5 - 4	v=0	[87012]
	21481.312	(0.022)	9/2 - 7/2	a	4 - 3	v=0	[87012]
	21484.710	(0.022)	9/2 - 7/2	b	5 - 4	v=0	[87012]
	21485.261	(0.025)	9/2 - 7/2	b	4 - 3	v=0	[87012]
	73993.8	(0.3)	31/2 - 29/2	a		v=0	[86024]
	73998.9	(0.3)	31/2 - 29/2	b		v=0	[86024]
	83541.5	(0.8)	35/2 - 33/2	a		v=0	[86024]
	83547.1	(0.6)	35/2 - 33/2	b		v=0	[86024]
	88315.2	(0.4)	37/2 - 35/2	a		v=0	[86024]
	88321.0	(0.4)	37/2 - 35/2	b		v=0	[86024]
	93089.0	(0.3)	39/2 - 37/2	a		v=0	[86024]
	93094.9	(0.4)	39/2 - 37/2	b		v=0	[86024]
	97862.6	(0.4)	41/2 - 39/2	a		v=0	[86024]
	97868.8	(0.4)	41/2 - 39/2	b		v=0	[86024]
	102635.7	(0.7)	43/2 - 41/2	a		v=0	[86024]
	102642.4	(0.7)	43/2 - 41/2	b		v=0	[86024]
	107409.91	(0.10)	45/2 - 43/2	a		v=0	[86004]
	107416.65	(0.10)	45/2 - 43/2	b		v=0	[86004]
	112183.49	(0.10)	47/2 - 45/2	a		v=0	[86004]
	112190.58	(0.10)	47/2 - 45/2	b		v=0	[86004]
	116957.11	(0.10)	49/2 - 47/2	a		v=0	[86004]
	116964.39	(0.10)	49/2 - 47/2	b		v=0	[86004]
	169464.50	(0.10)	71/2 - 69/2	a		v=0	[86004]
169475.49	(0.10)	71/2 - 69/2	b		v=0	[86004]	
183783.87	(0.10)	77/2 - 75/2	a		v=0	[86004]	
183796.03	(0.10)	77/2 - 75/2	b		v=0	[86004]	
188556.91	(0.10)	79/2 - 77/2	a		v=0	[86004]	
188569.50	(0.10)	79/2 - 77/2	b		v=0	[86004]	
CCCCCH ² Π _{3/2}	165785.43	(0.10)	69/2 - 67/2	a		v=0	[86004]
	165792.36	(0.10)	69/2 - 67/2	b		v=0	[86004]
	170588.58	(0.10)	71/2 - 69/2	a		v=0	[86004]
	170595.94	(0.10)	71/2 - 69/2	b		v=0	[86004]
	184997.07	(0.10)	77/2 - 75/2	a		v=0	[86004]
	185005.57	(0.10)	77/2 - 75/2	b		v=0	[86004]
	189799.43	(0.10)	79/2 - 77/2	a		v=0	[86004]
	189808.36	(0.10)	79/2 - 77/2	b		v=0	[86004]

Table 32.1. Rotational and centrifugal distortion constants for 1,4-pentadiyne. [81036]

Parameter	$\text{CH}_2(\text{CCH})_2$ ground state	$\text{CH}_2(\text{CCH})_2$ $\nu_{21} = 1$	$\text{CH}_2(\text{CCD})_2$ ground state
A'' (MHz)	19076.77(2) ^a	19300.82(11)	17408.3(112)
B'' (MHz)	2859.224(3)	2870.209(2)	2574.372(13)
C'' (MHz)	2520.801(3)	2524.646(5)	2270.134(13)
τ_1 (MHz)	0.2392(1)	0.2379(90)	0.2012(63)
τ_2 (MHz)	0.02182(1)	0.02491(38)	0.0207(89)
τ_3^b (MHz)	0.6068(11)	1.58(90)	1.25(220)
τ_{aaaa} (MHz)	-2.963(3)	-10.2(45)	-17.5(450)
τ_{bbbb} (MHz)	-0.01138(1)	-0.1296(146)	-0.01059(171)
τ_{cccc} (MHz)	-0.00317(2)	-0.00394(83)	-0.00316(57)

^aUncertainties are one standard deviation.^bValue determined by setting $R_6 = 0$.

TABLE 32.2. Microwave spectrum of 1,4-pentadiyne

C₅H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	J'(K ₋₁ ,K ₋₁) - J''(K ₊₁ ,K ₊₁)	Vib. state	Ref.
HCCCH ₂ CCH	16899.14	(0.20)	2(1, 1) - 2(0, 2)		[81036]
	18018.53	(0.20)	6(0, 6) - 5(1, 5)	1ν ₂₁	[81036]
	18100.37	(0.20)	6(0, 6) - 5(1, 5)		[81036]
	18143.73	(0.20)	4(1, 3) - 4(0, 4)		[81036]
	18396.02	(0.20)	4(1, 3) - 4(0, 4)	1ν ₂₁	[81036]
	19071.16	(0.20)	5(1, 4) - 5(0, 5)		[81036]
	19343.51	(0.20)	5(1, 4) - 5(0, 5)	1ν ₂₁	[81036]
	20225.36	(0.20)	6(1, 5) - 6(0, 6)		[81036]
	20523.09	(0.20)	6(1, 5) - 6(0, 6)	1ν ₂₁	[81036]
	21596.93	(0.20)	1(1, 1) - 0(0, 0)		[81036]
	21627.28	(0.20)	7(1, 6) - 7(0, 7)		[81036]
	21823.07	(0.20)	1(1, 1) - 0(0, 0)	1ν ₂₁	[81036]
	21956.17	(0.20)	7(1, 6) - 7(0, 7)	1ν ₂₁	[81036]
	23299.28	(0.20)	8(1, 7) - 8(0, 8)		[81036]
	23665.60	(0.20)	8(1, 7) - 8(0, 8)	1ν ₂₁	[81036]
	24192.14	(0.20)	7(0, 7) - 6(1, 6)	1ν ₂₁	[81036]
	24244.96	(0.20)	7(0, 7) - 6(1, 6)		[81036]
	25264.01	(0.20)	9(1, 8) - 9(0, 9)		[81036]
	25674.78	(0.20)	9(1, 8) - 9(0, 9)	1ν ₂₁	[81036]
	26638.85	(0.20)	2(1, 2) - 1(0, 1)		[81036]
	26872.62	(0.20)	2(1, 2) - 1(0, 1)	1ν ₂₁	[81036]
	27542.53	(0.20)	10(1, 9) - 10(0, 10)		[81036]
	28005.01	(0.20)	10(1, 9) - 10(0, 10)	1ν ₂₁	[81036]
	30152.26	(0.20)	11(1, 10) - 11(0, 11)		[81036]
	30419.34	(0.20)	8(0, 8) - 7(1, 7)	1ν ₂₁	[81036]
	30442.87	(0.20)	8(0, 8) - 7(1, 7)		[81036]
	30674.16	(0.20)	11(1, 10) - 11(0, 11)	1ν ₂₁	[81036]
	31513.62	(0.20)	3(1, 3) - 2(0, 2)		[81036]
	31751.77	(0.20)	3(1, 3) - 2(0, 2)	1ν ₂₁	[81036]
	36227.87	(0.20)	4(1, 4) - 3(0, 3)		[81036]
	36466.88	(0.20)	4(1, 4) - 3(0, 3)	1ν ₂₁	[81036]
	100496.36	(0.20)	19(1, 19) - 18(0, 18)		[81036]
	101169.15	(0.20)	26(4, 22) - 26(3, 23)		[81036]
	101278.05	(0.20)	20(0, 20) - 19(1, 19)		[81036]
	101333.49	(0.20)	22(1, 21) - 21(2, 20)		[81036]
	102758.06	(0.20)	12(2, 11) - 11(1, 10)		[81036]
	103791.43	(0.20)	27(2, 25) - 26(3, 24)		[81036]
	104876.70	(0.20)	24(4, 20) - 24(3, 21)		[81036]
	105081.94	(0.20)	25(2, 24) - 25(1, 25)		[81036]
	105120.35	(0.20)	20(1, 20) - 19(0, 19)		[81036]
	106230.55	(0.20)	13(2, 12) - 12(1, 11)		[81036]
	106273.67	(0.20)	27(1, 26) - 27(0, 27)		[81036]
	106496.20	(0.20)	23(4, 19) - 23(3, 20)		[81036]
	106664.48	(0.20)	21(0, 21) - 20(1, 20)		[81036]
	109584.52	(0.20)	14(2, 13) - 13(1, 12)		[81036]
	109808.00	(0.20)	21(1, 21) - 20(0, 20)		[81036]
	111968.50	(0.20)	18(4, 14) - 18(3, 15)		[81036]
	111991.90	(0.20)	22(0, 22) - 21(1, 21)		[81036]
	112209.61	(0.20)	22(0, 22) - 21(1, 21)	1ν ₂₁	[81036]
	113790.93	(0.20)	14(4, 10) - 14(3, 11)		[81036]
	114197.88	(0.20)	12(4, 8) - 12(3, 9)		[81036]
	114255.51	(0.20)	6(3, 3) - 5(2, 4)		[81036]
	114324.65	(0.20)	11(4, 7) - 11(3, 8)		[81036]
	114353.96	(0.20)	16(4, 13) - 16(3, 14)		[81036]
	114362.56	(0.20)	15(4, 12) - 15(3, 13)		[81036]
	114364.44	(0.20)	17(4, 14) - 17(3, 15)		[81036]
	114383.65	(0.20)	14(4, 11) - 14(3, 12)		[81036]
	114401.67	(0.20)	18(4, 15) - 18(3, 16)		[81036]
	114411.77	(0.20)	13(4, 10) - 13(3, 11)		[81036]
	114414.55	(0.20)	10(4, 6) - 10(3, 7)		[81036]
	114442.45	(0.20)	12(4, 9) - 12(3, 10)		[81036]
	114522.22	(0.20)	9(4, 6) - 9(3, 7)		[81036]
	114539.83	(0.20)	8(4, 5) - 8(3, 6)		[81036]
	114541.85	(0.20)	7(4, 3) - 7(3, 4)		[81036]
	114556.12	(0.20)	6(4, 2) - 6(3, 3)		[81036]
	114560.32	(0.20)	6(4, 3) - 6(3, 4)		[81036]
114563.05	(0.20)	5(4, 1) - 5(3, 2)		[81036]	

TABLE 32.2. Microwave spectrum of 1,4-pentadiyne — Continued

C₅H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{-1}) - J''(K_{+1}, K_{+1})$	Vib. state	Ref.
DCCCH ₂ CCD	114564.45	(0.20)	5(4, 2) - 5(3, 3)	1v ₂₁	[81036]
	114756.95	(0.20)	22(1,22) - 21(0,21)		[81036]
	116980.68	(0.20)	29(1,28) - 29(0,29)		[81036]
	117268.50	(0.20)	23(0,23) - 22(1,22)		[81036]
	122174.89	(0.20)	29(2,28) - 29(1,29)		[81036]
	122502.40	(0.20)	24(0,24) - 23(1,23)		[81036]
	18428.85	(0.20)	6(1, 5) - 6(0, 6)		[81036]
	19674.14	(0.20)	1(1, 1) - 0(0, 0)		[81036]
	19686.03	(0.20)	7(1, 6) - 7(0, 7)		[81036]
	21184.71	(0.20)	8(1, 7) - 8(0, 8)		[81036]
	22945.11	(0.20)	9(1, 8) - 9(0, 9)		[81036]
	24214.72	(0.20)	2(1, 2) - 1(0, 1)		[81036]
	24986.27	(0.20)	10(1, 9) - 10(0,10)		[81036]
	27194.30	(0.20)	8(0, 8) - 7(1, 7)		[81036]
	27323.91	(0.20)	11(1,10) - 11(0,11)		[81036]
	28604.97	(0.20)	3(1, 3) - 2(0, 2)		[81036]
	32804.24	(0.20)	9(0, 9) - 8(1, 8)		[81036]
	32850.84	(0.20)	4(1, 4) - 3(0, 3)		[81036]
	32928.62	(0.20)	13(1,12) - 13(0,13)		[81036]
	36199.12	(0.20)	14(1,13) - 14(0,14)		[81036]

Table 33.1. Molecular constants for 1,3-pentadiyne and deuterated isotopic species in the ground state.

Parameter	CH ₃ C ₄ H	CH ₃ C ₄ D	CD ₃ C ₄ H	CD ₃ C ₄ D
<u>Rotational Constants</u>				
B ₀ (MHz)	2035.74706(8)	1929.772(30)	1834.856(20)	1742.214(20)
D _{JK} (kHz)	19.8630(13)	18.3(1)	14.5(1)	13.5(1)
D _J (kHz)	0.086687(40)	0.06	0.1	0.1
H _{KJ} (Hz)	0.3278(37)			
H _{JK} (Hz)	0.03568(21)			
H _J (Hz)	0.0000130(66)			
Reference	[84035]	[55019]	[55019]	[55019]
<u>Dipole Moment</u> [85035]				
μ (D)	1.2071(10)			

Table 33.2. Rotational constants for 1,3-pentadiyne in the first excited vibrational state (v=1)^a and for various ¹³C substituted forms in the ground state.^b

Species	v	B _v (MHz)	q (MHz)	D _{JK} (kHz)	ζ	X ^a (kHz)
CH ₃ C ₄ H	1	2040.14(2)	2.104	20.0	0.9	0.15
CH ₃ C ₄ D	1	1933.86(2)	1.956	18.7	0.92	0.20
CD ₃ C ₄ H	1	1838.69(2)	1.804	14.6	0.9	0.23
CD ₃ C ₄ D	1	1745.80(2)	1.684	14.0	0.9	0.23
¹³ CH ₃ C ₄ H	0	1982.68(4)				
CH ₃ ¹³ CC ₃ H	0	2025.31(4)				
CH ₃ C ₂ ¹³ CCH	0	2018.96(4)				
CH ₃ C ₃ ¹³ CH	0	1980.22(4)				
¹³ CH ₃ C ₄ D	0	1879.93(4)				
CH ₃ ¹³ CC ₃ D	0	1919.42(4)				
CH ₃ C ₂ ¹³ CCD	0	1915.84(4)				
CH ₃ C ₃ ¹³ CD	0	1881.88(4)				

^aFrom reference [55019].^bFrom reference [57017].

TABLE 33.3. Microwave spectrum of methyl diacetylene

C₃H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	J' K ₋₁	-	J'' K ₊₁	Vib. state	Ref.
CH ₃ C ₂ H	20354.18	(0.10)	5(4)	-	4(4)		[55019]
	20355.55	(0.10)	5(3)	-	4(3)		[55019]
	20356.56	(0.10)	5(2)	-	4(2)		[55019]
	20357.226	(0.014)	5(1)	-	4(1)		[84036]
	20357.423	(0.014)	5(0)	-	4(0)		[84036]
	20390.87	(0.10)	5(+1)	-	4(+1)	1ν ₁ ℓ = +1	[55019]
	20399.69	(0.10)	5(+2)	-	4(+2)	1ν ₁ ℓ = -1	[55019]
	20399.69	(0.10)	5(+4)	-	4(+4)	1ν ₁ ℓ = +1	[55019]
	20400.64	(0.10)	5(+1)	-	4(+1)	1ν ₁ ℓ = -1	[55019]
	20400.64	(0.10)	5(+3)	-	4(+3)	1ν ₁ ℓ = +1	[55019]
	20401.24	(0.10)	5(+2)	-	4(+2)	1ν ₁ ℓ = +1	[55019]
	20401.24	(0.10)	5(0)	-	4(0)	1ν ₁ ℓ = +1	[55019]
	20411.95	(0.10)	5(+1)	-	4(+1)	1ν ₁ ℓ = +1	[55019]
	24422.83	(0.10)	6(5)	-	5(5)		[55019]
	24425.03	(0.10)	6(4)	-	5(4)		[55019]
	24426.69	(0.10)	6(3)	-	5(3)		[55019]
	24427.85	(0.10)	6(2)	-	5(2)		[55019]
	24428.652	(0.016)	6(1)	-	5(1)		[84036]
	24428.886	(0.016)	6(0)	-	5(0)		[84036]
	24469.11	(0.10)	6(+1)	-	5(+1)	1ν ₁ ℓ = +1	[55019]
	24475.95	(0.10)	6(+4)	-	5(+4)	1ν ₁ ℓ = -1	[55019]
	24479.62	(0.10)	6(+2)	-	5(+2)	1ν ₁ ℓ = -1	[55019]
	24479.62	(0.10)	6(+4)	-	5(+4)	1ν ₁ ℓ = +1	[55019]
	24480.78	(0.10)	6(+1)	-	5(+1)	1ν ₁ ℓ = -1	[55019]
	24480.78	(0.10)	6(+3)	-	5(+3)	1ν ₁ ℓ = +1	[55019]
	24481.52	(0.10)	6(+2)	-	5(+2)	1ν ₁ ℓ = +1	[55019]
	24481.52	(0.10)	6(0)	-	5(0)	1ν ₁ ℓ = +1	[55019]
	24494.38	(0.10)	6(+1)	-	5(+1)	1ν ₁ ℓ = +1	[55019]
	36630.24	(0.10)	9(6)	-	8(6)		[55019]
	36634.20	(0.10)	9(5)	-	8(5)		[55019]
	36637.49	(0.10)	9(4)	-	8(4)		[55019]
	36639.90	(0.10)	9(3)	-	8(3)		[55019]
	36641.70	(0.10)	9(2)	-	8(2)		[55019]
	36642.77	(0.10)	9(1)	-	8(1)		[55019]
	36643.08	(0.10)	9(0)	-	8(0)		[55019]
	36703.62	(0.10)	9(+1)	-	8(+1)	1ν ₁ ℓ = +1	[55019]
	36710.05	(0.10)	9(+5)	-	8(+5)	1ν ₁ ℓ = -1	[55019]
	36713.83	(0.10)	9(+4)	-	8(+4)	1ν ₁ ℓ = -1	[55019]
	36716.90	(0.10)	9(+5)	-	8(+5)	1ν ₁ ℓ = +1	[55019]
	36716.90	(0.10)	9(+3)	-	8(+3)	1ν ₁ ℓ = -1	[55019]
	36719.38	(0.10)	9(+4)	-	8(+4)	1ν ₁ ℓ = +1	[55019]
	36719.38	(0.10)	9(+2)	-	8(+2)	1ν ₁ ℓ = -1	[55019]
	36721.20	(0.10)	9(+3)	-	8(+3)	1ν ₁ ℓ = +1	[55019]
	36721.20	(0.10)	9(+1)	-	8(+1)	1ν ₁ ℓ = -1	[55019]
	36722.30	(0.10)	9(+2)	-	8(+2)	1ν ₁ ℓ = +1	[55019]
	36722.30	(0.10)	9(0)	-	8(0)	1ν ₁ ℓ = +1	[55019]
	36741.46	(0.10)	9(+1)	-	8(+1)	1ν ₁ ℓ = +1	[55019]
	40695.10	(0.10)	10(7)	-	9(7)		[55019]
	40700.28	(0.10)	10(6)	-	9(6)		[55019]
	40704.62	(0.10)	10(5)	-	9(5)		[55019]
	40708.20	(0.10)	10(4)	-	9(4)		[55019]
	40710.96	(0.10)	10(3)	-	9(3)		[55019]
	40712.96	(0.10)	10(2)	-	9(2)		[55019]
	40714.14	(0.10)	10(1)	-	9(1)		[55019]
	40714.56	(0.10)	10(0)	-	9(0)		[55019]
	44750.52	(0.10)	11(9)	-	10(9)		[55019]
	44764.52	(0.10)	11(7)	-	10(7)		[55019]
	44770.20	(0.10)	11(6)	-	10(6)		[55019]
	44775.04	(0.10)	11(5)	-	10(5)		[55019]
	44778.98	(0.10)	11(4)	-	10(4)		[55019]
	44782.02	(0.10)	11(3)	-	10(3)		[55019]
	44784.16	(0.10)	11(2)	-	10(2)		[55019]
	44785.48	(0.10)	11(1)	-	10(1)		[55019]
	44785.92	(0.10)	11(0)	-	10(0)		[55019]
	146238.500	(0.005)	36(15)	-	35(15)		[84035]
	146279.553	(0.005)	36(14)	-	35(14)		[84035]
	146317.722	(0.005)	36(13)	-	35(13)		[84035]

TABLE 33.3. Microwave spectrum of methyl diacetylene — Continued

C₃H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' K_{-1}$	-	$J'' K_{+1}$	Vib. state	Ref.
CH ₃ C ₂ D	146353.109	(0.005)	36(12)	-	35(12)		[84035]
	146385.722	(0.005)	36(11)	-	35(11)		[84035]
	146415.497	(0.005)	36(10)	-	35(10)		[84035]
	146442.465	(0.005)	36(9)	-	35(9)		[84035]
	146466.609	(0.005)	36(8)	-	35(8)		[84035]
	146487.914	(0.005)	36(7)	-	35(7)		[84035]
	146506.397	(0.005)	36(6)	-	35(6)		[84035]
	146522.046	(0.005)	36(5)	-	35(5)		[84035]
	146534.848	(0.005)	36(4)	-	35(4)		[84035]
	146544.810	(0.005)	36(3)	-	35(3)		[84035]
	146551.920	(0.005)	36(2)	-	35(2)		[84035]
	146556.188	(0.005)	36(1)	-	35(1)		[84035]
	146557.620	(0.005)	36(0)	-	35(0)		[84035]
	19296.08	(0.10)	5(3)	-	4(3)		[55019]
	19296.98	(0.10)	5(2)	-	4(2)		[55019]
	19297.52	(0.10)	5(1)	-	4(1)		[55019]
	19297.70	(0.10)	5(0)	-	4(0)		[55019]
	19328.94	(0.10)	5(+1)	-	4(+1)	1ν ₁ ℓ = +1	[55019]
	19335.80	(0.10)	5(+3)	-	4(+3)	1ν ₁ ℓ = -1	[55019]
	19337.14	(0.10)	5(+2)	-	4(+2)	1ν ₁ ℓ = -1	[55019]
	19337.14	(0.10)	5(+4)	-	4(+4)	1ν ₁ ℓ = +1	[55019]
	19338.02	(0.10)	5(+1)	-	4(+1)	1ν ₁ ℓ = -1	[55019]
	19338.02	(0.10)	5(+3)	-	4(+3)	1ν ₁ ℓ = +1	[55019]
	19338.58	(0.10)	5(0)	-	4(0)	1ν ₁ ℓ = +1	[55019]
	19338.58	(0.10)	5(+2)	-	4(+2)	1ν ₁ ℓ = +1	[55019]
	19348.50	(0.10)	5(+1)	-	4(+1)	1ν ₁ ℓ = +1	[55019]
	23151.67	(0.10)	6(5)	-	5(5)		[55019]
	23153.71	(0.10)	6(4)	-	5(4)		[55019]
	23155.25	(0.10)	6(3)	-	5(3)		[55019]
	23156.34	(0.10)	6(2)	-	5(2)		[55019]
	23156.99	(0.10)	6(1)	-	5(1)		[55019]
	23157.21	(0.10)	6(0)	-	5(0)		[55019]
	23194.67	(0.10)	6(+1)	-	5(+1)	1ν ₁ ℓ = +1	[55019]
	23202.96	(0.10)	6(+3)	-	5(+3)	1ν ₁ ℓ = -1	[55019]
	23204.48	(0.10)	6(+2)	-	5(+2)	1ν ₁ ℓ = -1	[55019]
	23204.48	(0.10)	6(+4)	-	5(+4)	1ν ₁ ℓ = +1	[55019]
	23205.54	(0.10)	6(+3)	-	5(+3)	1ν ₁ ℓ = +1	[55019]
	23205.54	(0.10)	6(+1)	-	5(+1)	1ν ₁ ℓ = -1	[55019]
	23206.23	(0.10)	6(+2)	-	5(+2)	1ν ₁ ℓ = +1	[55019]
	23206.23	(0.10)	6(0)	-	5(0)	1ν ₁ ℓ = +1	[55019]
	23218.17	(0.10)	6(+1)	-	5(+1)	1ν ₁ ℓ = +1	[55019]
	42434.89	(0.10)	11(7)	-	10(7)		[55019]
	42440.20	(0.10)	11(6)	-	10(6)		[55019]
	42444.61	(0.10)	11(5)	-	10(5)		[55019]
	42448.24	(0.10)	11(4)	-	10(4)		[55019]
	42451.03	(0.10)	11(3)	-	10(3)		[55019]
	42453.05	(0.10)	11(2)	-	10(2)		[55019]
	42454.25	(0.10)	11(1)	-	10(1)		[55019]
	42454.66	(0.10)	11(0)	-	10(0)		[55019]
	46298.32	(0.10)	12(6)	-	11(6)		[55019]
	46303.13	(0.10)	12(5)	-	11(5)		[55019]
	46307.07	(0.10)	12(4)	-	11(4)		[55019]
	46310.16	(0.10)	12(3)	-	11(3)		[55019]
	46312.36	(0.10)	12(2)	-	11(2)		[55019]
	46313.66	(0.10)	12(1)	-	11(1)		[55019]
	46314.11	(0.10)	12(0)	-	11(0)		[55019]
46389.10	(0.10)	12(+1)	-	11(+1)	1ν ₁ ℓ = +1	[55019]	
46389.94	(0.10)	12(+8)	-	11(+8)	1ν ₁ ℓ = +1	[55019]	
46390.82	(0.10)	12(+6)	-	11(+6)	1ν ₁ ℓ = -1	[55019]	
46396.24	(0.10)	12(+7)	-	11(+7)	1ν ₁ ℓ = +1	[55019]	
46396.90	(0.10)	12(+5)	-	11(+5)	1ν ₁ ℓ = -1	[55019]	
46405.40	(0.10)	12(+3)	-	11(+3)	1ν ₁ ℓ = -1	[55019]	
46405.40	(0.10)	12(+5)	-	11(+5)	1ν ₁ ℓ = +1	[55019]	
46408.54	(0.10)	12(+2)	-	11(+2)	1ν ₁ ℓ = -1	[55019]	
46408.54	(0.10)	12(+4)	-	11(+4)	1ν ₁ ℓ = +1	[55019]	
46410.76	(0.10)	12(+3)	-	11(+3)	1ν ₁ ℓ = +1	[55019]	
46410.76	(0.10)	12(+1)	-	11(+1)	1ν ₁ ℓ = -1	[55019]	

TABLE 33.3. Microwave spectrum of methyl diacetylene — Continued

C₃H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	J' K ₋₁	-	J'' K ₊₁	Vib. state	Ref.
CD ₃ C ₂ H	46411.82	(0.10)	12(0)	-	11(0)	1ν ₁ ℓ = +1	[55019]
	46412.42	(0.10)	12(+2)	-	11(+2)	1ν ₁ ℓ = +1	[55019]
	46436.04	(0.10)	12(+1)	-	11(+1)	1ν ₁ ℓ = +1	[55019]
	25684.57	(0.10)	7(4)	-	6(4)		[55019]
	25686.05	(0.10)	7(3)	-	6(3)		[55019]
	25687.03	(0.10)	7(2)	-	6(2)		[55019]
	25687.66	(0.10)	7(1)	-	6(1)		[55019]
	25687.84	(0.10)	7(0)	-	6(0)		[55019]
	33010.35	(0.10)	9(8)	-	8(8)		[55019]
	33014.30	(0.10)	9(7)	-	8(7)		[55019]
	33017.74	(0.10)	9(6)	-	8(6)		[55019]
	33020.60	(0.10)	9(5)	-	8(5)		[55019]
	33022.94	(0.10)	9(4)	-	8(4)		[55019]
	33024.77	(0.10)	9(3)	-	8(3)		[55019]
	33026.08	(0.10)	9(2)	-	8(2)		[55019]
	33026.86	(0.10)	9(1)	-	8(1)		[55019]
	33027.09	(0.10)	9(0)	-	8(0)		[55019]
	33080.20	(0.10)	9(+1)	-	8(+1)	1ν ₁ ℓ = +1	[55019]
	33083.30	(0.10)	9(+8)	-	8(+8)	1ν ₁ ℓ = +1	[55019]
	33087.11	(0.10)	9(+5)	-	8(+5)	1ν ₁ ℓ = -1	[55019]
	33089.98	(0.10)	9(+4)	-	8(+4)	1ν ₁ ℓ = -1	[55019]
	33092.23	(0.10)	9(+3)	-	8(+3)	1ν ₁ ℓ = -1	[55019]
	33092.23	(0.10)	9(+5)	-	8(+5)	1ν ₁ ℓ = +1	[55019]
	33094.08	(0.10)	9(+2)	-	8(+2)	1ν ₁ ℓ = -1	[55019]
	33094.08	(0.10)	9(+4)	-	8(+4)	1ν ₁ ℓ = +1	[55019]
	33095.39	(0.10)	9(+1)	-	8(+1)	1ν ₁ ℓ = -1	[55019]
	33095.39	(0.10)	9(+3)	-	8(+3)	1ν ₁ ℓ = +1	[55019]
	33096.06	(0.10)	9(0)	-	8(0)	1ν ₁ ℓ = +1	[55019]
	33096.27	(0.10)	9(+2)	-	8(+2)	1ν ₁ ℓ = +1	[55019]
	33112.67	(0.10)	9(+1)	-	8(+1)	1ν ₁ ℓ = +1	[55019]
	44023.24	(0.10)	12(6)	-	11(6)		[55019]
	44027.08	(0.10)	12(5)	-	11(5)		[55019]
	44030.18	(0.10)	12(4)	-	11(4)		[55019]
44032.64	(0.10)	12(3)	-	11(3)		[55019]	
44034.42	(0.10)	12(2)	-	11(2)		[55019]	
44035.48	(0.10)	12(1)	-	11(1)		[55019]	
44035.80	(0.10)	12(0)	-	11(0)		[55019]	
CD ₃ C ₂ D	24386.10	(0.10)	7(5)	-	6(5)		[55019]
	24387.83	(0.10)	7(4)	-	6(4)		[55019]
	24389.17	(0.10)	7(3)	-	6(3)		[55019]
	24390.12	(0.10)	7(2)	-	6(2)		[55019]
	24390.68	(0.10)	7(1)	-	6(1)		[55019]
	24390.85	(0.10)	7(0)	-	6(0)		[55019]
	34822.04	(0.10)	10(9)	-	9(9)		[55019]
	34826.67	(0.10)	10(8)	-	9(8)		[55019]
	34830.70	(0.10)	10(7)	-	9(7)		[55019]
	34834.26	(0.10)	10(6)	-	9(6)		[55019]
	34837.21	(0.10)	10(5)	-	9(5)		[55019]
	34839.63	(0.10)	10(4)	-	9(4)		[55019]
	34841.53	(0.10)	10(3)	-	9(3)		[55019]
	34842.86	(0.10)	10(2)	-	9(2)		[55019]
	34843.65	(0.10)	10(1)	-	9(1)		[55019]
	34843.89	(0.10)	10(0)	-	9(0)		[55019]
	34898.93	(0.10)	10(+1)	-	9(+1)	1ν ₁ ℓ = +1	[55019]
	34909.06	(0.10)	10(+4)	-	9(+4)	1ν ₁ ℓ = -1	[55019]
	34911.46	(0.10)	10(+3)	-	9(+3)	1ν ₁ ℓ = -1	[55019]
	34911.46	(0.10)	10(+5)	-	9(+5)	1ν ₁ ℓ = +1	[55019]
	34913.28	(0.10)	10(+4)	-	9(+4)	1ν ₁ ℓ = +1	[55019]
	34913.28	(0.10)	10(+2)	-	9(+2)	1ν ₁ ℓ = -1	[55019]
	34914.63	(0.10)	10(+1)	-	9(+1)	1ν ₁ ℓ = -1	[55019]
	34914.63	(0.10)	10(+3)	-	9(+3)	1ν ₁ ℓ = +1	[55019]
	34915.35	(0.10)	10(0)	-	9(0)	1ν ₁ ℓ = +1	[55019]
	34915.70	(0.10)	10(+2)	-	9(+2)	1ν ₁ ℓ = +1	[55019]
	34932.59	(0.10)	10(+1)	-	9(+1)	1ν ₁ ℓ = +1	[55019]
45284.10	(0.10)	13(6)	-	12(6)		[55019]	
45287.88	(0.10)	13(5)	-	12(5)		[55019]	
45291.10	(0.10)	13(4)	-	12(4)		[55019]	

TABLE 33.3. Microwave spectrum of methyl diacetylene — Continued

C₅H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	J' K ₋₁ - J'' K ₊₁	Vib. state	Ref.
	45293.56	(0.10)	13(3) - 12(3)		[55019]
	45295.30	(0.10)	13(2) - 12(2)		[55019]
	45296.40	(0.10)	13(1) - 12(1)		[55019]
	45296.66	(0.10)	13(0) - 12(0)		[55019]

Table 34.1. Molecular constants for cyclopentadiene.

Parameter	Value
<u>Rotational Constants</u> [present analysis]	
A'' (MHz)	6426.1205(69)
B'' (MHz)	8225.6602(12)
C'' (MHz)	4271.4441(31)
τ ₁ (MHz)	-0.02703(603)
τ ₂ (MHz)	-0.00822(203)
τ ₃ ^a (MHz)	1.37(20)
τ _{aaaa} (MHz)	-0.01347(199)
τ _{bbbb} (MHz)	-0.01484(228)
<u>Dipole Moment</u> [65030]	
μ _b	0.419(4) D
<u>Magnetic Constants</u> [70065]	
g _{aa}	-0.0700(3) μ _N
g _{bb}	-0.0827(3) μ _N
g _{cc}	0.0385(2) μ _N
2χ _{aa} -χ _{bb} -χ _{cc}	+30.7(3)x10 ⁻⁶ erg/(G ² ·mol)
2χ _{bb} -χ _{aa} -χ _{cc}	+37.8(3)x10 ⁻⁶ erg/(G ² ·mol)
Q _{aa}	1.4(4)x10 ⁻²⁶ esu·cm ²
Q _{bb}	3.7(4)x10 ⁻²⁶ esu·cm ²
Q _{cc}	-5.1(5)x10 ⁻²⁶ esu·cm ²

^aValue determined by setting R_g = 0.Table 34.2. Rotational constants for ¹³C substituted cyclopentadiene. [65030]

Parameter	¹³ C ₁ ^a	¹³ C ₂	¹³ C ₃
A (MHz)	8226.04(3)	8420.02(3)	8345.11(3)
B (MHz)	8219.46(3)	8040.41(3)	8108.70(3)
C (MHz)	4217.76(3)	4119.40(3)	4119.07(3)

^aAtom numbering is as follows: $\overline{C_1H_2C_2H=C_3HC_4H=C_5H}$ where C₃ and C₄ and C₅ and C₅ are equivalent.

TABLE 34.3. Microwave spectrum of cyclopentadiene

C₅H₆


Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.		
$\text{CH}_2\text{CHCHCHCH}$ 	11869.990	(0.050)	2(1, 1) - 2(0, 2)	[65030]		
	12697.560	(0.008)	1(1, 1) - 0(0, 0)	[70065]		
	19658.900	(0.100)	7(5, 2) - 7(4, 3)	[56018]		
	19914.700	(0.100)	6(4, 2) - 6(3, 3)	[56018]		
	20085.220	(0.100)	5(3, 2) - 5(2, 3)	[56018]		
	20186.990	(0.050)	4(2, 2) - 4(1, 3)	[65030]		
	20239.702	(0.020)	3(1, 2) - 3(0, 3)	[70065]		
	20276.615	(0.020)	3(2, 2) - 3(1, 3)	[70065]		
	20291.300	(0.100)	12(12, 1) - 12(11, 2)	[56018]		
	20296.530	(0.050)	4(3, 2) - 4(2, 3)	[65030]		
	20336.680	(0.050)	5(4, 2) - 5(3, 3)	[65030]		
	20406.400	(0.100)	6(5, 2) - 6(4, 3)	[56018]		
	21032.498	(0.009)	2(0, 2) - 1(1, 1)	[70065]		
	21240.397	(0.010)	2(1, 2) - 1(0, 1)	[70065]		
	$\text{HC}-\text{CH}$ $\parallel \quad \parallel$ $\text{HC} \quad \text{CH}$ $\backslash \quad /$ CH_2	29549.691	(0.010)	2(2, 1) - 1(1, 0)	[70065]	
29678.259		(0.020)	3(0, 3) - 2(1, 2)	[70065]		
29685.863		(0.010)	3(1, 3) - 2(0, 2)	[70065]		
¹³ CH ₂ CHCHCHCH		11965.43	(0.05)	5(4, 1) - 5(4, 2)	[65030]	
		11981.95	(0.05)	4(3, 1) - 4(3, 2)	[65030]	
		11995.20	(0.05)	3(2, 1) - 3(2, 2)	[65030]	
		12024.86	(0.05)	2(2, 1) - 2(0, 2)	[65030]	
		12034.69	(0.05)	3(3, 1) - 3(1, 2)	[65030]	
		12064.32	(0.05)	5(3, 2) - 5(5, 1)	[65030]	
		20872.74	(0.05)	2(1, 2) - 1(1, 1)	[65030]	
		28876.14	(0.05)	2(1, 1) - 1(1, 0)	[65030]	
		29311.54	(0.05)	3(3, 0) - 2(2, 0)	[65030]	
		37311.57	(0.05)	3(2, 2) - 2(2, 1)	[65030]	
		37331.25	(0.05)	3(1, 2) - 2(1, 1)	[65030]	
		CH ₂ ¹³ CHCHCHCH	11489.92	(0.05)	2(1, 1) - 2(0, 2)	[65030]
	19418.77		(0.05)	5(3, 2) - 5(2, 3)	[65030]	
	19754.90		(0.05)	4(2, 2) - 4(1, 3)	[65030]	
	20070.25		(0.05)	3(2, 2) - 3(1, 3)	[65030]	
20281.58	(0.05)		5(4, 2) - 5(3, 3)	[65030]		
20671.73	(0.05)		2(0, 2) - 1(1, 1)	[65030]		
$\text{CH}_2\text{CH}^{13}\text{CHCHCH}$ $\text{CH}_2^{13}\text{CHCHCHCH}$	20755.44		(0.05)	2(0, 2) - 1(1, 1)	[65030]	
	21078.23		(0.05)	2(1, 2) - 1(0, 1)	[65030]	
	29309.79		(0.05)	3(0, 3) - 2(1, 2)	[65030]	
	29337.87		(0.05)	3(1, 3) - 2(0, 2)	[65030]	
	29479.47		(0.05)	2(2, 1) - 1(1, 0)	[65030]	
	CH ₂ CH ¹³ CHCHCH		11679.34	(0.05)	2(1, 1) - 2(0, 2)	[65030]
			19920.14	(0.05)	4(2, 2) - 4(1, 3)	[65030]
			19779.11	(0.05)	5(3, 2) - 5(2, 3)	[65030]
			20045.53	(0.05)	3(2, 2) - 3(1, 3)	[65030]
		20129.60	(0.05)	5(4, 2) - 5(3, 3)	[65030]	
		20991.80	(0.05)	2(0, 2) - 1(0, 1)	[65030]	
		21002.32	(0.05)	2(1, 2) - 1(0, 1)	[65030]	
		28545.06	(0.05)	2(1, 1) - 1(1, 0)	[65030]	
		29254.40	(0.05)	2(2, 1) - 1(1, 0)	[65030]	
		29326.24	(0.05)	3(1, 3) - 2(0, 2)	[65030]	

Table 35.1. Molecular constants for 1-penten-3-yne.

Parameter	CH ₂ =CHCCCH ₃	
A (GHz)	36.8(17)	
B (MHz)	2126.90(10)	
C (MHz)	2026.32(10)	
Dipole Moment [71045]		
μ_a (D)	0.571(2)	
μ_b (D)	0.334(41)	

TABLE 35.2. Microwave spectrum of 1-penten-3-yne

C₅H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
CH ₂ CHCCCH ₃	8205.87	(0.10)	2(1, 2) - 1(1, 1)	[71045]
	8306.08	(0.10)	2(0, 2) - 1(0, 1)	[71045]
	8407.04	(0.10)	2(1, 1) - 1(1, 0)	[71045]
	12308.71	(0.10)	3(1, 3) - 2(1, 2)	[71045]
	12458.68	(0.10)	3(0, 3) - 2(0, 2)	[71045]
	12610.44	(0.10)	3(1, 2) - 2(1, 1)	[71045]
	16411.31	(0.10)	4(1, 4) - 3(1, 3)	[71045]
	16813.73	(0.10)	4(1, 3) - 3(1, 2)	[71045]
	20513.72	(0.10)	5(1, 5) - 4(1, 4)	[71045]
	21016.46	(0.10)	5(1, 4) - 4(1, 3)	[71045]
	24615.90	(0.10)	6(1, 6) - 5(1, 5)	[71045]
	25219.37	(0.10)	6(1, 5) - 5(1, 4)	[71045]
	29421.74	(0.10)	7(1, 6) - 6(1, 5)	[71045]

Table 36.1. Rotational constants and dipole moment for normal and deuterated cyclopropylacetylene.

Parameter	C ₃ H ₅ C≡CH	C ₃ H ₅ C≡CD
A (MHz)	15722.90(133)	15653.(63)
B (MHz)	3360.006(4)	3139.67(2)
C (MHz)	3192.703(4)	2997.95(2)
μ_a (D)	0.891(10)	
μ_c (D)	0.048(10)	
References	[83051] [72062]	[72062]

Table 36.2. Rotational constants for ¹³C isotopic forms of cyclopropylacetylene.

Isotopic Species	A (MHz)	B (MHz)	C (MHz)
Rotational Constants [83051]			
CH ₂ CH ₂ ¹³ CHCCH (1- ¹³ C)	15538.76(3604)	3350.53(2)	3190.99(2)
CH ₂ ¹³ CH ₂ CHCCH (2- ¹³ C)	15426.69(2363)	3319.58(2)	3146.32(2)
CH ₂ CH ₂ CH ¹³ CCH (4- ¹³ C)	15681.92(2400)	3334.68(2)	3170.33(2)
CH ₂ CH ₂ CHC ¹³ CH (5- ¹³ C)	15772.14(2171)	3254.22(2)	3097.90(1)

TABLE 36.3. Microwave spectrum of cyclopropylacetylene

C₃H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.	
CH ₂ CH ₂ CH(CCH) □	12938.25	(0.05)	2(1, 2) - 1(1, 1)	[72062]	
	13103.80	(0.05)	2(0, 2) - 1(0, 1)	[72062]	
	13272.72	(0.05)	2(1, 1) - 1(1, 0)	[72062]	
	19406.24	(0.05)	3(1, 3) - 2(1, 2)	[72062]	
	19651.50	(0.05)	3(0, 3) - 2(0, 2)	[72062]	
	H ₂ C-CH ₂	19658.18	(0.05)	3(2, 2) - 2(2, 1)	[72062]
		19664.80	(0.05)	3(2, 1) - 2(2, 0)	[72062]
	∨	19908.02	(0.05)	3(1, 2) - 2(1, 1)	[72062]
	CH	25872.90	(0.05)	4(1, 4) - 3(1, 3)	[72062]
		26193.97	(0.05)	4(0, 4) - 3(0, 3)	[72062]
	C	26209.56	(0.05)	4(2, 3) - 3(2, 2)	[72062]
		26214.59	(0.05)	4(3, 1) - 3(3, 0)	[72062]
	CH	26214.59	(0.05)	4(3, 2) - 3(3, 1)	[72062]
		26226.20	(0.05)	4(2, 2) - 3(2, 1)	[72062]
	26541.96	(0.05)	4(1, 3) - 3(1, 2)	[72062]	
	28051.36	(0.05)	18(1,17) - 18(1,18)	[83051]	
	31026.02	(0.05)	19(1,18) - 19(1,19)	[83051]	
	34110.84	(0.05)	20(1,19) - 20(1,20)	[83051]	
	37294.97	(0.05)	21(1,20) - 21(1,21)	[83051]	
CH ₂ CH ₂ CH(CCD) □	12133.54	(0.05)	2(1, 2) - 1(1, 1)	[72062]	
	12274.03	(0.05)	2(0, 2) - 1(0, 1)	[72062]	
	12416.95	(0.05)	2(1, 1) - 1(1, 0)	[72062]	
	18199.50	(0.05)	3(1, 3) - 2(1, 2)	[72062]	
	18408.02	(0.05)	3(0, 3) - 2(0, 2)	[72062]	
	18412.89	(0.05)	3(2, 2) - 2(2, 1)	[72062]	
	18417.59	(0.05)	3(2, 1) - 2(2, 0)	[72062]	
	18624.67	(0.05)	3(1, 2) - 2(1, 1)	[72062]	
	CH ₂ CH ₂ ¹³ CH(CCH) □	32302.18	(0.05)	5(1, 5) - 4(1, 4)	[83051]
		32704.17	(0.05)	5(2, 4) - 4(2, 3)	[83051]
32711.22		(0.05)	5(4, 1) - 4(4, 0)	[83051]	
32712.90		(0.05)	5(3, 3) - 4(3, 2)	[83051]	
32735.28		(0.05)	5(2, 3) - 4(2, 2)	[83051]	
33099.62		(0.05)	5(1, 4) - 4(1, 3)	[83051]	
38758.14		(0.05)	6(1, 5) - 5(1, 5)	[83051]	
39241.85		(0.05)	6(2, 5) - 5(2, 4)	[83051]	
39296.24		(0.05)	6(2, 4) - 5(2, 3)	[83051]	
39714.88		(0.05)	6(1, 5) - 5(1, 4)	[83051]	
CH ₂ ¹³ CH ₂ CH(CCH) □	31888.41	(0.05)	5(1, 5) - 4(1, 4)	[83051]	
	32292.78	(0.05)	5(0, 5) - 4(0, 4)	[83051]	
	32325.48	(0.05)	5(2, 4) - 4(2, 3)	[83051]	
	32333.81	(0.05)	5(4, 1) - 4(4, 0)	[83051]	
	32362.44	(0.05)	5(2, 3) - 4(2, 2)	[83051]	
	38261.00	(0.05)	6(1, 6) - 5(1, 5)	[83051]	
	38730.90	(0.05)	6(0, 6) - 5(0, 5)	[83051]	
	38786.90	(0.05)	6(2, 5) - 5(2, 4)	[83051]	
	38851.26	(0.05)	6(2, 4) - 5(2, 3)	[83051]	
	39299.92	(0.05)	6(1, 5) - 5(1, 4)	[83051]	
	CH ₂ CH ₂ CH(¹³ CCH) □	32107.28	(0.05)	5(1, 5) - 4(1, 4)	[83051]
		32521.56	(0.05)	5(2, 4) - 4(2, 3)	[83051]
32554.05		(0.05)	5(2, 3) - 4(2, 2)	[83051]	
38524.22		(0.05)	6(1, 6) - 5(1, 5)	[83051]	
38973.20		(0.05)	6(0, 6) - 5(0, 5)	[83051]	
39022.64		(0.05)	6(2, 5) - 5(2, 4)	[83051]	
39039.00		(0.05)	6(3, 4) - 5(3, 3)	[83051]	
39079.52		(0.05)	6(2, 4) - 5(2, 3)	[83051]	
CH ₂ CH ₂ CH(C ¹³ CH) □		31363.66	(0.05)	5(1, 5) - 4(1, 4)	[83051]
		31731.59	(0.05)	5(0, 5) - 4(0, 4)	[83051]
	31757.48	(0.05)	5(2, 4) - 4(2, 3)	[83051]	
	31765.63	(0.05)	5(3, 3) - 4(3, 2)	[83051]	
	31786.68	(0.05)	5(2, 3) - 4(2, 2)	[83051]	
	32145.08	(0.05)	5(1, 4) - 4(1, 3)	[83051]	
	37632.28	(0.05)	6(1, 6) - 5(1, 5)	[83051]	
	38061.62	(0.05)	6(0, 6) - 5(0, 5)	[83051]	
	38106.06	(0.05)	6(2, 5) - 5(2, 4)	[83051]	
	38116.33	(0.05)	6(5, 1) - 5(5, 0)	[83051]	
	38117.60	(0.05)	6(4, 2) - 5(4, 1)	[83051]	
	38120.38	(0.05)	6(3, 4) - 5(3, 3)	[83051]	
	38157.09	(0.05)	6(2, 4) - 5(2, 3)	[83051]	

Table 37.1. Molecular constants for
2-methyl-1-buten-3-yne.

Parameter	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_2=\text{CC}=\text{CH} \end{array}$
<u>Rotation-Internal Rotation Constants [present]</u>	
A (MHz)	9359.699(32)
B (MHz)	4013.514(20)
C (MHz)	2854.749(11)
Δ_{JK} (kHz)	15.9(12)
δ_J (kHz)	0.45(18)
δ_K (kHz)	5.9(30)
I_α (u \AA^2)	3.133 ^a
θ	59.2 ^a
V_3 (cm^{-1})	2016.(40)
<u>Electric Dipole Moment [69067]</u>	
μ_a (D)	0.448(15)
μ_b (D)	0.248(10)

^aAssumed value.

TABLE 37.2. Microwave spectrum of 2-methyl-1-buten-3-yne

C₅H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Sym.	Ref.
CH ₂ C(CH ₃)CCH	10108.5	(0.1)	3(1, 2) - 3(0, 3)	A	[69067]
	12214.6	(0.1)	1(1, 1) - 0(0, 0)	A	[69067]
	12578.0	(0.1)	2(1, 2) - 1(1, 1)	A	[69067]
CH ₃	13567.9	(0.1)	2(0, 2) - 1(0, 1)	A	[69067]
	14680.8	(0.1)	4(2, 2) - 4(1, 3)	A	[69067]
H ₂ C=CCCH	14895.3	(0.1)	2(1, 1) - 1(1, 0)	A	[69067]
	14955.9	(0.1)	5(2, 3) - 5(1, 4)	A	[69067]
	15235.5	(0.1)	3(2, 1) - 3(1, 2)	A	[69067]
	17924.0	(0.1)	2(1, 2) - 1(0, 1)	A	[69067]
	18767.9	(0.1)	3(1, 3) - 2(1, 2)	A	[69067]
	19942.73	(0.10)	8(2, 6) - 8(2, 7)	E	[69067]
	19943.1	(0.1)	8(2, 6) - 8(2, 7)	A	[69067]
	19952.3	(0.1)	3(0, 3) - 2(0, 2)	A	[69067]
	20604.5	(0.1)	3(2, 2) - 2(2, 1)	A	[69067]
	21256.9	(0.1)	3(2, 1) - 2(2, 0)	A	[69067]
	22228.4	(0.1)	3(1, 2) - 2(1, 1)	A	[69067]
	23124.0	(0.1)	3(1, 3) - 2(0, 2)	A	[69067]
	23332.5	(0.1)	8(2, 6) - 8(1, 7)	A	[69067]
	23332.23	(0.10)	8(2, 6) - 8(1, 7)	E	[69067]
	23800.6	(0.1)	6(1, 5) - 6(0, 6)	E	[69067]
	23800.9	(0.1)	6(1, 5) - 6(0, 6)	A	[69067]
	24859.8	(0.1)	4(1, 4) - 3(1, 3)	A	[69067]
	25964.7	(0.1)	4(0, 4) - 3(0, 3)	A	[69067]
	27340.5	(0.1)	4(2, 3) - 3(2, 2)	A	[69067]
	27767.8	(0.1)	4(3, 2) - 3(3, 1)	A	[69067]
	27859.38	(0.10)	4(3, 1) - 3(3, 0)	E	[69067]
	27859.6	(0.1)	4(3, 1) - 3(3, 0)	A	[69067]
	28847.7	(0.1)	4(2, 2) - 3(2, 1)	A	[69067]
	29402.6	(0.1)	4(1, 3) - 3(1, 2)	A	[69067]
	30849.6	(0.1)	5(1, 5) - 4(1, 4)	A	[69067]
	30933.5	(0.1)	2(2, 1) - 1(1, 0)	A	[69067]
	30961.4	(0.1)	5(3, 3) - 5(2, 4)	A	[69067]
	31692.5	(0.1)	5(0, 5) - 4(0, 4)	A	[69067]
	32261.1	(0.1)	2(2, 0) - 1(1, 1)	A	[69067]
	32268.1	(0.1)	6(3, 4) - 6(2, 5)	A	[69067]
	33966.5	(0.1)	5(2, 4) - 4(2, 3)	A	[69067]
	34713.0	(0.1)	5(4, 2) - 4(4, 1)	A	[69067]
	34714.12	(0.10)	5(4, 2) - 4(4, 1)	E	[69067]
	34721.14	(0.10)	5(4, 1) - 4(4, 0)	E	[69067]
	34722.4	(0.1)	5(4, 1) - 4(4, 0)	A	[69067]
	34775.2	(0.1)	5(3, 3) - 4(3, 2)	A	[69067]
	35087.3	(0.1)	5(3, 2) - 4(3, 1)	A	[69067]
	36606.2	(0.1)	5(2, 3) - 4(2, 2)	A	[69067]
	36606.08	(0.10)	5(2, 3) - 4(2, 2)	E	[69067]

Table 38.1. Molecular constants for *cis*-3-penten-1-yne.

Parameter	CH ₃ CH=CHC≡CH
A (MHz)	11792.088(63)
B (MHz)	3388.222(18)
C (MHz)	2672.221(20)
Δ _J (MHz)	0.00230(16)
Δ _{JK} (MHz)	-0.0132(12)
δ _J (MHz)	0.00088(27)
<u>Internal Rotation Constants</u>	
I _α (u Å ²)	3.16 (assumed)
θ	76.8(2)°
s	31.63
V ₃ (cm ⁻¹)	389.3(10)

TABLE 38.2. Microwave spectrum of *cis*-3-pentene-1-yneC₅H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	J'(K ₋₁ ,K ₊₁) - J''(K ₋₁ ,K ₊₁)	Sym.	Ref.
CH ₃ CHCHCCH	9880.18	(0.05)	2(1, 1) - 2(0, 2)	A	[71049]
	12076.72	(0.05)	2(0, 2) - 1(0, 1)	E	[71049]
	12077.43	(0.05)	2(0, 2) - 1(0, 1)	A	[71049]
	18006.55	(0.05)	3(0, 3) - 2(0, 2)	E	[71049]
	18007.53	(0.05)	3(0, 3) - 2(0, 2)	A	[71049]
	18182.21	(0.05)	3(2, 2) - 2(2, 1)	A	[71049]
	18185.19	(0.05)	3(2, 2) - 2(2, 1)	E	[71049]
	18351.03	(0.05)	3(2, 1) - 2(2, 0)	E	[71049]
	18356.41	(0.05)	3(2, 1) - 2(2, 0)	A	[71049]
	19226.25	(0.05)	3(1, 2) - 2(1, 1)	E	[71049]
	19227.91	(0.05)	3(1, 2) - 2(1, 1)	A	[71049]
	22726.46	(0.05)	4(1, 4) - 3(1, 3)	E	[71049]
	22727.19	(0.05)	4(1, 4) - 3(1, 3)	A	[71049]
	23812.19	(0.05)	4(0, 4) - 3(0, 3)	E	[71049]
	23813.31	(0.05)	4(0, 4) - 3(0, 3)	A	[71049]
	24634.62	(0.05)	4(2, 2) - 3(2, 1)	E	[71049]
	24637.25	(0.05)	4(2, 2) - 3(2, 1)	A	[71049]
	31033.36	(0.05)	5(2, 3) - 4(2, 2)	E	[71049]
	31036.14	(0.05)	5(2, 3) - 4(2, 2)	A	[71049]
	31880.08	(0.05)	5(1, 4) - 4(1, 3)	E	[71049]
31882.59	(0.05)	5(1, 4) - 4(1, 3)	A	[71049]	

Table 39.1. Molecular constants for bicyclo[2.1.0]pent-2-ene.

Parameter	CHCH=CHCHCH ₂	
<u>Rotational Constants</u>		
A (MHz)	10811.65(11)	
B (MHz)	6517.883(3)	
C (MHz)	5216.287(3)	
<u>Dipole Moment</u>		
μ_a	0.398(1)	D
μ_c	0.025(2)	D
<u>Zeeman Constants</u>		
g_{aa}	-0.0046(18)	μ_N
g_{bb}	-0.0342(11)	μ_N
g_{cc}	-0.0218(12)	μ_N
$2\chi_{aa}-\chi_{bb}-\chi_{cc}$	-14.9(11) $\times 10^{-6}$ erg/(G ² ·mol)	
$-\chi_{aa}+2\chi_{bb}-\chi_{cc}$	7.8(15) $\times 10^{-6}$ erg/(G ² ·mol)	
Reference	[70064]	

TABLE 39.2. Microwave spectrum of bicyclo [2.1.0]pent-2-ene

C₅H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
CHCHCHCHCH ₂	11734.19	(0.10)	1(0, 1) - 0(0, 0)	[70064]
	12799.54	(0.10)	4(1, 3) - 4(1, 4)	[70064]
	22166.75	(0.10)	2(1, 2) - 1(1, 1)	[70064]
	23214.68	(0.10)	2(0, 2) - 1(0, 1)	[70064]
	24769.92	(0.10)	2(1, 1) - 1(1, 0)	[70064]
$\begin{array}{c} \text{HC}=\text{CH} \\ \quad \\ \text{HC}-\text{CH} \\ \vee \\ \text{CH}_2 \end{array}$	33104.42	(0.10)	3(1, 3) - 2(1, 2)	[70064]
	34245.47	(0.10)	3(0, 3) - 2(0, 2)	[70064]
	35202.53	(0.10)	3(2, 2) - 2(2, 1)	[70064]
	36159.53	(0.10)	3(2, 1) - 2(2, 0)	[70064]
	36977.55	(0.10)	3(1, 2) - 2(1, 1)	[70064]

Table 39.1A. Molecular constants for 1,2,3-pentatriene

Parameter	CH ₂ =C=C=CHCH ₃
A (MHz)	29788.(20)
B (MHz)	2212.987(5)
C (MHz)	2085.026(4)
D _J (kHz)	0.446(22)
D _{JK} (kHz)	-33.95(5)
I _α (u Å ²)	3.10 ^a
θ	44.4°
V ₃ (cm ⁻¹)	468.5(7)
<u>Electric Dipole Moment</u> [87021]	
μ_a (D)	0.50(5)
μ_b (D)	0.122(3)

TABLE 39.2.a. Microwave spectrum of 1,2,3-pentatriene

C₃H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_-,K_+) - J''(K_-,K_+)$	Sym.	Ref.
CH ₂ CCCHCH ₃	12702.10	(0.50)	3(1, 3) - 2(1, 2)	A	[87021]
	12892.32	(0.50)	3(0, 3) - 2(0, 2)	A	[87021]
	13086.13	(0.50)	3(1, 2) - 2(1, 1)	A	[87021]
	16935.46	(0.50)	4(1, 4) - 3(1, 3)	A	[87021]
	16936.44	(0.50)	4(1, 4) - 3(1, 3)	E	[87021]
	17187.55	(0.50)	4(0, 4) - 3(0, 3)	A	[87021]
	17447.55	(0.50)	4(1, 3) - 3(1, 2)	A	[87021]
	21168.31	(0.50)	5(1, 5) - 4(1, 4)	A	[87021]
	21168.78	(0.50)	5(1, 5) - 4(1, 4)	E	[87021]
	25400.87	(0.50)	6(1, 6) - 5(1, 5)	A	[87021]
	25772.42	(0.50)	6(0, 6) - 5(0, 5)	A	[87021]
	25787.51	(0.50)	6(2, 5) - 5(2, 4)	A	[87021]
	25794.00	(0.50)	6(3, 3) - 5(3, 2)	A	[87021]
	25794.00	(0.50)	6(3, 4) - 5(3, 3)	A	[87021]
	25795.79	(0.50)	6(4, 3) - 5(4, 2)	A	[87021]
	25803.00	(0.50)	6(2, 4) - 5(2, 3)	A	[87021]
	26168.79	(0.50)	6(1, 5) - 5(1, 4)	A	[87021]
	29632.40	(0.50)	7(1, 7) - 6(1, 6)	A	[87021]
	30060.51	(0.50)	7(0, 7) - 6(0, 6)	E	[87021]
	30060.81	(0.50)	7(0, 7) - 6(0, 6)	A	[87021]
	30084.21	(0.50)	7(2, 6) - 6(2, 5)	A	[87021]
	30093.50	(0.50)	7(3, 4) - 6(3, 3)	A	[87021]
	30093.50	(0.50)	7(3, 5) - 6(3, 4)	A	[87021]
	30093.50	(0.50)	7(2, 6) - 6(2, 5)	E	[87021]
	30095.35	(0.50)	7(4, 4) - 6(4, 3)	A	[87021]
	30099.20	(0.50)	7(5, 3) - 6(5, 2)	A	[87021]
	30099.20	(0.50)	7(2, 5) - 6(2, 4)	E	[87021]
	30103.80	(0.50)	7(6, 2) - 6(6, 1)	A	[87021]
	30109.00	(0.50)	7(2, 5) - 6(2, 4)	A	[87021]
	30527.48	(0.50)	7(1, 6) - 6(1, 5)	E	[87021]
	30528.32	(0.50)	7(1, 6) - 6(1, 5)	A	[87021]
	33863.25	(0.50)	8(1, 8) - 7(1, 7)	A	[87021]
	34345.69	(0.50)	8(0, 8) - 7(0, 7)	E	[87021]
	34346.20	(0.50)	8(0, 8) - 7(0, 7)	A	[87021]
	34380.18	(0.50)	8(2, 7) - 7(2, 6)	A	[87021]
	34391.20	(0.50)	8(2, 7) - 7(2, 6)	E	[87021]
	34393.60	(0.50)	8(3, 6) - 7(3, 5)	A	[87021]
	34395.15	(0.50)	8(4, 5) - 7(4, 4)	A	[87021]
	34399.07	(0.50)	8(5, 4) - 7(5, 3)	A	[87021]
	34404.40	(0.50)	8(6, 3) - 7(6, 2)	A	[87021]
	34405.62	(0.50)	8(2, 6) - 7(2, 5)	E	[87021]
	34411.09	(0.50)	8(7, 2) - 7(7, 1)	A	[87021]
	34417.48	(0.50)	8(2, 6) - 7(2, 5)	A	[87021]
	34886.13	(0.50)	8(1, 7) - 7(1, 6)	E	[87021]
	34887.00	(0.50)	8(1, 7) - 7(1, 6)	A	[87021]
	38093.20	(0.50)	9(1, 9) - 8(1, 8)	A	[87021]
	38627.51	(0.50)	9(0, 9) - 8(0, 8)	E	[87021]
	38627.96	(0.50)	9(0, 9) - 8(0, 8)	A	[87021]
	38675.60	(0.50)	9(2, 8) - 8(2, 7)	A	[87021]
	38686.75	(0.50)	9(2, 8) - 8(2, 7)	E	[87021]
	38693.88	(0.50)	9(3, 6) - 8(3, 5)	A	[87021]
	38693.88	(0.50)	9(3, 7) - 8(3, 6)	A	[87021]
	38695.00	(0.50)	9(4, 5) - 8(4, 4)	A	[87021]
	38695.00	(0.50)	9(4, 6) - 8(4, 5)	A	[87021]
	38699.10	(0.50)	9(5, 5) - 8(5, 4)	A	[87021]
	38705.19	(0.50)	9(6, 4) - 8(6, 3)	A	[87021]
	38712.48	(0.50)	9(7, 3) - 8(7, 2)	A	[87021]
	38716.74	(0.50)	9(2, 7) - 8(2, 6)	E	[87021]
	38721.10	(0.50)	9(8, 2) - 8(8, 1)	A	[87021]
	38728.78	(0.50)	9(2, 7) - 8(2, 6)	A	[87021]
	39243.83	(0.50)	9(1, 8) - 8(1, 7)	E	[87021]
	39244.73	(0.50)	9(1, 8) - 8(1, 7)	A	[87021]

Table 40.1. Molecular constants for trans-isoprene
(2-methyl-1,3-butadiene).

Parameter	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_2=\text{CCH}=\text{CH}_2 \end{array}$
<u>Rotational Constants</u> [present]	
A'' (MHz)	8527.025(7)
B'' (MHz)	4175.529(17)
C'' (MHz)	2852.170(6)
τ_1 (kHz)	-29.4(3)
τ_2 (kHz)	-6.64(96)
τ_3 (kHz)	100.7(102)
τ_{bbbb} (kHz)	-4.97(82)
<u>Derived Constants</u>	
D _J (kHz)	6.22(52)
D _{JK} (kHz)	5.49(53)
δ_J (kHz)	0.31(5)
<u>Internal Rotation Constants</u> [69058]	
I_α (u Å ²)	3.132
θ	6.1730
V_3 (cm ⁻¹)	917.(35)
<u>Electric Dipole Moment</u> [64028]	
μ_a (D)	0.035(2)
μ_b (D)	0.25(1)
<u>Magnetic Constants</u> [70065]	
g_{aa}	-0.0621(13) μ_N
g_{bb}	-0.0339(16) μ_N
g_{cc}	0.0080(16) μ_N
$2\chi_{aa}-\chi_{bb}-\chi_{cc}$	16.7(12) $\times 10^{-6}$ erg/(G ² ·mol)
$2\chi_{bb}-\chi_{aa}-\chi_{cc}$	19.2(10) $\times 10^{-6}$ erg/(G ² ·mol)
Q_{aa}	1.7(2.2) $\times 10^{-26}$ esu·cm ²
Q_{bb}	3.3(2.3) $\times 10^{-26}$ esu·cm ²
Q_{cc}	-5.0(3.2) $\times 10^{-26}$ esu·cm ²

TABLE 40.2. Microwave spectrum of isoprene

C₅H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
<i>t</i> -CH ₂ C(CH ₃)CHCH ₂	16189.000	(0.100)	6(2, 4) - 6(1, 5)	[69058]
	17083.468	(0.007)	2(1, 2) - 1(0, 1)	[70065]
	20473.700	(0.100)	7(2, 5) - 7(1, 6)	[69058]
	22236.310	(0.070)	3(1, 3) - 2(0, 2)	[70065]
	22694.040	(0.050)	4(3, 1) - 4(2, 2)	[64028]
	24013.660	(0.050)	3(3, 0) - 3(2, 1)	[64028]
	24734.710	(0.100)	10(4, 6) - 10(3, 7)	[64028]
	25048.550	(0.100)	11(4, 7) - 11(3, 8)	[64028]
	25214.870	(0.100)	3(3, 1) - 3(2, 2)	[64028]
	25619.790	(0.100)	5(2, 4) - 5(1, 5)	[64028]
	25852.100	(0.050)	4(3, 2) - 4(2, 3)	[64028]
	26022.200	(0.100)	9(4, 5) - 9(3, 6)	[64028]
	26169.410	(0.100)	8(2, 6) - 8(1, 7)	[64028]
	26261.080	(0.100)	10(3, 7) - 10(2, 8)	[64028]
	27027.700	(0.200)	5(3, 3) - 5(2, 4)	[64028]
	27158.000	(0.050)	4(1, 4) - 3(0, 3)	[64028]
	27349.430	(0.100)	12(4, 8) - 12(3, 9)	[64028]
	28433.200	(0.008)	2(2, 1) - 1(1, 0)	[70065]
	30014.840	(0.030)	2(2, 0) - 1(1, 1)	[70065]
	32217.260	(0.050)	11(3, 8) - 11(2, 9)	[64028]
	32717.030	(0.050)	9(2, 7) - 9(1, 8)	[64028]
	38201.000	(0.100)	8(1, 7) - 8(0, 8)	[69058]
	39172.800	(0.100)	12(3, 9) - 12(2, 10)	[69058]
	39487.400	(0.100)	10(2, 8) - 10(1, 9)	[69058]

Table 41.1. Molecular constants for 3-methyl-1-butyne (isopropyl acetylene).

Parameter	HC≡CCH(CH ₃) ₂ [Present]	Parameter	HC≡CCH(CH ₃) ₂ [73079]
A'' (MHz)	7969.49123(2168)	A (MHz)	7969.48(2)
B'' (MHz)	3828.80099(293)	B (MHz)	3828.801(2)
C'' (MHz)	2833.23999(258)	C (MHz)	2833.216(2)
τ ₁ (MHz)	-50.1343(10727)	D _J (MHz)	-2.29(17)×10 ⁻³
τ ₂ (MHz)	-10.6737(3265)	D _{JK} (MHz)	-71.0(35)×10 ⁻³
τ ₃ ^a (MHz)	202.82(8)	D _K (MHz)	-0.1128(38)
τ _{aaaa} (MHz)	-22.248(3856)	D _{wj} (MHz)	0.89(4)×10 ⁻⁶
τ _{bbbb} (MHz)	-4.43347(23010)	D _{wk} (MHz)	23.2(10)×10 ⁻⁶
τ _{cccc} (MHz)	-0.83960(28223)		
<u>Electric Dipole Moment</u>			
		μ _a (D)	0.684(8)
		μ _c (D)	0.227(4)

^aThe value of τ₃ is fixed by setting R_ε = 0.

Table 41.2. Rotational constants for the excited vibrational states and isotopic species of 3-methyl-1-butyne. [73079]

Species	A (MHz)	B (MHz)	C (MHz)
(CH ₃) ₂ CHCCH ν ₁₉	8035.7(5)	3833.19(2)	2837.93(2)
(CH ₃) ₂ CHCCH ν ₂₃	7963.4(11)	3825.45(4)	2830.30(3)
(CH ₃) ₂ CHCCH ν ₂₄	7916.7(4)	3840.43(2)	2832.66(2)
(CH ₃) ₂ CHCCD	7957.2(5)	3553.60(1)	2681.19(1)
¹³ CH ₃ (CH ₃)CHCCH	7776.4(12)	3791.51(4)	2788.91(4)
¹³ CH ₃ (CH ₃)CHCCD	7763.0(7)	3519.01(2)	2640.07(2)

TABLE 41.3. Microwave spectrum of 3-methyl-1-butyne

C₅H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
HCCCH(CH ₃) ₂	9191.84	(0.05)	9(3, 6) - 9(3, 7)		[73079]
	9212.10	(0.05)	21(7,14) - 21(7,15)		[73079]
	9495.56	(0.05)	37(12,25) - 37(12,26)		[73079]
	9662.71	(0.05)	18(6,12) - 18(6,13)		[73079]
	9762.66	(0.05)	12(4, 8) - 12(4, 9)		[73079]
	9878.95	(0.05)	15(5,10) - 15(5,11)		[73079]
	12316.45	(0.10)	2(1, 2) - 1(1, 1)	1ν ₂₃	[73079]
	12328.44	(0.05)	2(1, 2) - 1(1, 1)		[73079]
	12338.49	(0.10)	2(1, 2) - 1(1, 1)	1ν ₂₄	[73079]
	12347.50	(0.10)	2(1, 2) - 1(1, 1)	1ν ₁₉	[73079]
	13152.73	(0.10)	2(0, 2) - 1(0, 1)	1ν ₂₃	[73079]
	13165.12	(0.05)	2(0, 2) - 1(0, 1)		[73079]
	13181.40	(0.10)	2(0, 2) - 1(0, 1)	1ν ₂₄	[73079]
	13185.60	(0.10)	2(0, 2) - 1(0, 1)	1ν ₁₉	[73079]
	13698.44	(0.05)	25(8,17) - 25(8,18)		[73079]
	14046.18	(0.05)	10(3, 7) - 10(3, 8)		[73079]
	14306.83	(0.10)	2(1, 1) - 1(1, 0)	1ν ₂₃	[73079]
	14319.54	(0.05)	2(1, 1) - 1(1, 0)		[73079]
	14337.59	(0.10)	2(1, 1) - 1(1, 0)	1ν ₁₉	[73079]
	14354.05	(0.10)	2(1, 1) - 1(1, 0)	1ν ₂₄	[73079]
	14483.38	(0.05)	22(7,15) - 22(7,16)		[73079]
	14912.90	(0.05)	13(4, 9) - 13(4,10)		[73079]
	14987.18	(0.05)	38(12,26) - 38(12,27)		[73079]
	15013.64	(0.05)	19(6,13) - 19(6,14)		[73079]
	16492.40	(0.05)	35(11,24) - 35(11,25)		[73079]
	17672.43	(0.05)	8(2, 6) - 8(2, 7)		[73079]
	18382.19	(0.10)	3(1, 3) - 2(1, 2)	1ν ₂₃	[73079]
	18400.14	(0.05)	3(1, 3) - 2(1, 2)		[73079]
	18411.92	(0.10)	3(1, 3) - 2(1, 2)	1ν ₂₄	[73079]
	18429.21	(0.10)	3(1, 3) - 2(1, 2)	1ν ₁₉	[73079]
	19270.66	(0.05)	29(9,20) - 29(9,21)		[73079]
	19356.99	(0.10)	3(0, 3) - 2(0, 2)	1ν ₂₃	[73079]
	19375.50	(0.05)	3(0, 3) - 2(0, 2)		[73079]
	19387.25	(0.10)	3(0, 3) - 2(0, 2)	1ν ₂₄	[73079]
	19410.52	(0.10)	3(0, 3) - 2(0, 2)	1ν ₁₉	[73079]
	19804.13	(0.05)	11(3, 8) - 11(3, 9)		[73079]
	19967.23	(0.10)	3(2, 2) - 2(2, 1)	1ν ₂₃	[73079]
	19985.73	(0.05)	3(2, 2) - 2(2, 1)		[73079]
	20013.20	(0.10)	3(2, 2) - 2(2, 1)	1ν ₁₉	[73079]
	20019.11	(0.10)	3(2, 2) - 2(2, 1)	1ν ₂₄	[73079]
	20399.12	(0.05)	26(8,18) - 26(8,19)		[73079]
	20577.23	(0.10)	3(2, 1) - 2(2, 0)	1ν ₂₃	[73079]
	20596.18	(0.05)	3(2, 1) - 2(2, 0)		[73079]
	20616.10	(0.10)	3(2, 1) - 2(2, 0)	1ν ₁₉	[73079]
	20651.26	(0.10)	3(2, 1) - 2(2, 0)	1ν ₂₄	[73079]
	21097.58	(0.05)	14(4,10) - 14(4,11)		[73079]
	21241.86	(0.05)	23(7,16) - 23(7,17)		[73079]
	21351.52	(0.10)	3(1, 2) - 2(1, 1)	1ν ₂₃	[73079]
	21370.70	(0.05)	3(1, 2) - 2(1, 1)		[73079]
	21399.29	(0.10)	3(1, 2) - 2(1, 1)	1ν ₁₉	[73079]
	21418.07	(0.10)	3(1, 2) - 2(1, 1)	1ν ₂₄	[73079]
	21692.90	(0.05)	17(5,12) - 17(5,13)		[73079]
	21705.95	(0.05)	20(6,14) - 20(6,15)		[73079]
	23463.37	(0.05)	9(2, 7) - 9(2, 8)		[73079]
	24357.57	(0.10)	4(1, 4) - 3(1, 3)	1ν ₂₃	[73079]
	24381.54	(0.05)	4(1, 4) - 3(1, 3)		[73079]
	24392.33	(0.10)	4(1, 4) - 3(1, 3)	1ν ₂₄	[73079]
	24421.95	(0.10)	4(1, 4) - 3(1, 3)	1ν ₁₉	[73079]
	25066.38	(0.05)	7(1, 6) - 7(1, 7)		[73079]
	25229.96	(0.10)	4(0, 4) - 3(0, 3)	1ν ₂₃	[73079]
	25254.89	(0.05)	4(0, 4) - 3(0, 3)		[73079]
	25255.50	(0.10)	4(0, 4) - 3(0, 3)	1ν ₂₄	[73079]
	25306.02	(0.10)	4(0, 4) - 3(0, 3)	1ν ₁₉	[73079]
	26523.24	(0.05)	4(2, 3) - 3(2, 2)		[73079]
	27417.30	(0.05)	30(9,21) - 30(9,22)		[73079]
	30271.75	(0.05)	5(1, 5) - 4(1, 4)		[73079]
	30904.28	(0.05)	5(0, 5) - 4(0, 4)		[73079]

TABLE 41.3. Microwave spectrum of 3-methyl-1-butyne

C₄H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
DCCCH(CH ₃) ₂	31726.59	(0.05)	40(12,28) - 40(12,29)		[73079]
	32957.16	(0.05)	5(2, 4) - 4(2, 3)		[73079]
	33707.38	(0.05)	5(3, 3) - 4(3, 2)		[73079]
	34929.40	(0.05)	5(1, 4) - 4(1, 3)		[73079]
	11597.26	(0.05)	2(1, 2) - 1(1, 1)		[73079]
	12352.45	(0.05)	2(0, 2) - 1(0, 1)		[73079]
	13342.11	(0.05)	2(1, 1) - 1(1, 0)		[73079]
	17326.93	(0.05)	3(1, 3) - 2(1, 2)		[73079]
	18248.91	(0.05)	3(0, 3) - 2(0, 2)		[73079]
	18704.40	(0.05)	3(2, 2) - 2(2, 1)		[73079]
	19159.90	(0.05)	3(2, 1) - 2(2, 0)		[73079]
	19934.19	(0.05)	3(1, 2) - 2(1, 1)		[73079]
	22986.83	(0.05)	4(1, 4) - 3(1, 3)		[73079]
	23875.36	(0.05)	4(0, 4) - 3(0, 3)		[73079]
	24847.35	(0.05)	4(2, 3) - 3(2, 2)		[73079]
	25146.66	(0.05)	4(3, 2) - 3(3, 1)		[73079]
	25205.58	(0.05)	4(3, 1) - 3(3, 0)		[73079]
25910.64	(0.05)	4(2, 2) - 3(2, 1)		[73079]	
26417.43	(0.05)	4(1, 3) - 3(1, 2)		[73079]	
HCCCH(¹³ CH ₃)(CH ₃)	19103.66	(0.10)	3(0, 3) - 2(0, 2)		[73079]
	21130.99	(0.10)	3(1, 2) - 2(1, 1)		[73079]
	24029.73	(0.10)	4(1, 4) - 3(1, 3)		[73079]
	24875.35	(0.10)	4(0, 4) - 3(0, 3)		[73079]
DCCCH(¹³ CH ₃)(CH ₃)	26191.10	(0.10)	4(2, 3) - 3(2, 2)		[73079]
	19712.79	(0.10)	3(1, 2) - 2(1, 1)		[73079]
	22661.99	(0.10)	4(1, 4) - 3(1, 3)		[73079]
	23528.99	(0.10)	4(0, 4) - 3(0, 3)		[73079]
	24540.12	(0.10)	4(2, 3) - 3(2, 2)		[73079]
	25646.71	(0.10)	4(2, 2) - 3(2, 1)		[73079]
26113.32	(0.10)	4(1, 3) - 3(1, 2)		[73079]	

Table 42.1. Molecular constants for the ground vibrational state of trans- and gauche-1-pentyne.

Parameter	trans-1-pentyne	gauche-1-pentyne
<u>Rotational Constants</u> [present]		
A'' (MHz)	23382.(66)	9921.116(21)
B'' (MHz)	2230.560(15)	3172.7689(36)
C'' (MHz)	2116.362(15)	2634.0128(36)
τ_1 (MHz)	0.0423(75)	0.03355(90)
τ_2 (MHz)	0.00247(53)	0.002203(202)
τ_3^a (MHz)	0.6(6)	0.472(6)
τ_{aaaa} (MHz)	---	-0.1777(116)
τ_{bbbb} (MHz)	-0.00166(70)	-0.018440(115)
τ_{cccc} (MHz)	-0.00149(65)	-0.004336(140)
<u>Centrifugal Distortion Constants</u> [71046]		
D _J (MHz)	0.00038(4)	0.0022(3)
D _{JK} (MHz)	-0.013(1)	-0.016(2)
D _K (MHz)	---	0.45(5)
<u>Electric Dipole Moment</u> [71046]		
μ_a (D)	0.8385(5)	0.687(2)
μ_b (D)	0.158(7)	0.317(4)
μ_c (D)		0.07(2)

^aThe value of τ_3 is fixed by setting $R_6 = 0$.

Table 42.2. Molecular constants for excited vibrational states of trans- and gauche-1-pentyne. [72063]

Species	Vibrational State ^a	A (MHz)	B (MHz)	C (MHz)	E (cm ⁻¹)
trans-1-pentyne	$\nu_{33}=1$	(22200)	2231.75	2121.08	106(10)
	$\nu_{33}=2$	(21500)	2233.09	2125.94	213(25)
	$\nu_{33}=3$	(20500)	2234.66	2130.97	330(30)
	$\nu_{33}=4$	(19500)	2236.32	2136.16	426(30)
	$\nu_{32}=1$	(23800)	2235.63	2118.28	166(15)
	$\nu_{32}=2$	(23900)	2240.58	2120.13	---
	$\nu_{33}=1, \nu_{32}=1$	(22700)	2236.33	2123.07	---
	$\nu_{31}=1$	(23000)	2228.39	2114.99	253(20)
	$\nu_{33}=1, \nu_{31}=1$	(20400)	2229.88	2119.39	---
gauche-1-pentyne	$\nu_{33}=1$	9974.64	3165.12	2629.18	114(10)
	$\nu_{33}=2$	10032.33	3156.99	2624.26	223(25)
	$\nu_{33}=3$	10092.15	3148.34	2619.26	323(30)
	$\nu_{33}=4$	(10163)	3138.43	2613.71	425(30)
	$\nu_{32}=1$	9948.04	3175.51	2634.81	177(15)
	$\nu_{32}=2$	(9968)	3178.12	2635.47	---
	$\nu_{33}=1, \nu_{32}=1$	10000.17	3167.50	2629.93	---
	$\nu_{31}=1$	9881.04	3174.83	2634.09	250(20)

^aThe vibrational modes are: ν_{33} (C₃-C₄ torsion), ν_{32} (C-C≡C bend) and ν_{31} (methyl internal rotation).

TABLE 42.3. Microwave spectrum of 1-pentyne

C₅H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
g-CH ₃ CH ₂ CH ₂ CCH	8768.50	(0.10)	3(1, 2) - 3(0, 3)		[71046]
	10084.55	(0.10)	4(1, 3) - 4(0, 4)		[71046]
	10120.25	(0.10)	4(1, 3) - 4(0, 4)	1ν ₃₂	[72063]
	10122.95	(0.10)	4(1, 3) - 4(0, 4)	1ν ₃₃	[72063]
	11074.77	(0.10)	2(1, 2) - 1(1, 1)		[71046]
	11582.48	(0.10)	2(0, 2) - 1(0, 1)		[71046]
	11589.40	(0.10)	2(0, 2) - 1(0, 1)	1ν ₃₂	[72063]
	11810.61	(0.10)	5(1, 4) - 4(2, 3)		[72063]
	11857.64	(0.10)	5(1, 4) - 5(0, 5)	1ν ₃₁	[72063]
	11874.15	(0.10)	5(1, 4) - 5(0, 5)		[71046]
	11898.20	(0.10)	5(1, 4) - 5(0, 5)	1ν ₃₃	[72063]
	11916.45	(0.10)	5(1, 4) - 5(0, 5)	1ν ₃₂	[72063]
	11922.78	(0.10)	5(1, 4) - 5(0, 5)	2ν ₃₃	[72063]
	11945.35	(0.10)	5(1, 4) - 5(0, 5)	3ν ₃₃	[72063]
	12095.20	(0.10)	2(1, 1) - 1(1, 0)	2ν ₃₃	[72063]
	12124.46	(0.10)	2(1, 1) - 1(1, 0)	1ν ₃₃	[72063]
	12152.19	(0.10)	2(1, 1) - 1(1, 0)		[71046]
	12158.56	(0.10)	2(1, 1) - 1(1, 0)		[72063]
	12161.30	(0.10)	2(1, 1) - 1(1, 0)	1ν ₃₂	[72063]
	12555.12	(0.10)	1(1, 1) - 0(0, 0)		[72063]
	14193.40	(0.10)	6(1, 5) - 6(0, 6)	1ν ₃₁	[72063]
	14196.15	(0.10)	6(1, 5) - 6(0, 6)		[72063]
	14201.46	(0.10)	6(1, 5) - 6(0, 6)	1ν ₃₃	[72063]
	14204.87	(0.10)	6(1, 5) - 6(0, 6)	2ν ₃₃	[72063]
	16526.44	(0.10)	3(1, 3) - 2(1, 2)	2ν ₃₃	[72063]
	16560.41	(0.10)	3(1, 3) - 2(1, 2)	1ν ₃₃	[72063]
	16593.31	(0.10)	3(1, 3) - 2(1, 2)		[71046]
	16601.03	(0.10)	3(1, 3) - 2(1, 2)	1ν ₃₂	[72063]
	17039.24	(0.10)	7(1, 6) - 7(0, 7)	2ν ₃₃	[72063]
	17060.75	(0.10)	7(1, 6) - 7(0, 7)	1ν ₃₃	[72063]
	17077.75	(0.10)	7(1, 6) - 7(0, 7)		[72063]
	17139.20	(0.10)	7(1, 6) - 7(0, 7)	1ν ₃₂	[72063]
	17225.03	(0.10)	3(0, 3) - 2(0, 2)	2ν ₃₃	[72063]
	17261.72	(0.10)	3(0, 3) - 2(0, 2)	1ν ₃₃	[72063]
	17296.83	(0.10)	3(0, 3) - 2(0, 2)		[71046]
	17301.65	(0.10)	3(0, 3) - 2(0, 2)	1ν ₃₁	[72063]
	17307.04	(0.10)	3(0, 3) - 2(0, 2)	1ν ₃₂	[72063]
	17385.64	(0.10)	4(0, 4) - 3(1, 3)		[72063]
	17420.52	(0.10)	3(2, 2) - 2(2, 1)		[71046]
	17538.13	(0.10)	7(2, 5) - 7(1, 6)		[72063]
	17543.60	(0.10)	3(2, 1) - 2(2, 0)		[71046]
	17713.02	(0.10)	6(2, 4) - 6(1, 5)		[72063]
	17786.38	(0.10)	8(2, 6) - 8(1, 7)		[72063]
	17823.15	(0.10)	2(1, 2) - 1(0, 1)		[72063]
	18024.05	(0.10)	3(1, 2) - 2(1, 1)	4ν ₃₃	[72063]
	18077.38	(0.10)	3(1, 2) - 2(1, 1)	3ν ₃₃	[72063]
	18123.42	(0.10)	3(1, 2) - 2(1, 1)	2ν ₃₃	[72063]
	18166.97	(0.10)	3(1, 2) - 2(1, 1)	1ν ₃₃	[72063]
	18178.72	(0.10)	3(1, 2) - 2(1, 1)	1ν ₃₃ , 1ν ₃₂	[72063]
	18202.18	(0.10)	5(2, 3) - 5(1, 4)		[72063]
	18208.31	(0.10)	3(1, 2) - 2(1, 1)		[71046]
	18217.38	(0.10)	3(1, 2) - 2(1, 1)	1ν ₃₁	[72063]
	18221.71	(0.10)	3(1, 2) - 2(1, 1)	1ν ₃₂	[72063]
	18234.40	(0.10)	3(1, 2) - 2(1, 1)	2ν ₃₂	[72063]
	18483.14	(0.10)	9(2, 7) - 9(1, 8)	1ν ₃₁	[72063]
	18545.57	(0.10)	9(2, 7) - 9(1, 8)		[71046]
	18612.19	(0.10)	9(2, 7) - 9(1, 8)	1ν ₃₂	[72063]
	18638.83	(0.10)	9(2, 7) - 9(1, 8)	1ν ₃₃	[72063]
	18805.36	(0.10)	10(2, 9) - 9(3, 6)		[72063]
	18879.00	(0.10)	4(2, 2) - 4(1, 3)		[72063]
	18890.46	(0.10)	8(1, 7) - 8(1, 8)		[72063]
	19102.56	(0.10)	12(2, 10) - 12(2, 11)		[72063]
	19610.92	(0.10)	3(2, 1) - 3(1, 2)		[72063]
	19886.12	(0.10)	10(2, 8) - 10(1, 9)		[72063]
	19939.97	(0.10)	10(2, 8) - 10(1, 9)	1ν ₃₃	[72063]
	19957.53	(0.10)	10(2, 8) - 10(1, 9)	1ν ₃₂	[72063]
	20275.50	(0.10)	2(2, 0) - 2(1, 1)		[72063]

TABLE 42.3. Microwave spectrum of 1-pentyne — Continued

C₅H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	20410.72	(0.10)	8(1, 7) - 8(0, 8)	2v ₃₃	[72063]
	20458.28	(0.10)	8(1, 7) - 8(0, 8)	1v ₃₃	[72063]
	20498.22	(0.10)	8(1, 7) - 8(0, 8)		[72063]
	20572.07	(0.10)	8(1, 7) - 8(0, 8)	1v ₃₂	[72063]
	21856.38	(0.10)	11(2, 9) - 11(1, 10)	1v ₃₁	[72063]
	21859.39	(0.10)	11(2, 9) - 11(1, 10)		[72063]
	21860.60	(0.10)	2(2, 1) - 2(1, 2)		[72063]
	21867.55	(0.10)	11(2, 9) - 11(1, 10)	1v ₃₃	[72063]
	21875.55	(0.10)	11(2, 9) - 11(1, 10)	2v ₃₃	[72063]
	21879.41	(0.10)	11(2, 9) - 11(1, 10)	3v ₃₃	[72063]
	21904.94	(0.10)	4(1, 4) - 3(1, 3)	4v ₃₃	[72063]
	21936.91	(0.10)	11(2, 9) - 11(1, 10)	1v ₃₂	[72063]
	21956.64	(0.10)	4(1, 4) - 3(1, 3)	3v ₃₃	[72063]
	22002.66	(0.10)	4(1, 4) - 3(1, 3)	2v ₃₃	[72063]
	22047.32	(0.10)	4(1, 4) - 3(1, 3)	1v ₃₃	[72063]
	22056.41	(0.10)	4(1, 4) - 3(1, 3)	1v ₃₃ , 1v ₃₂	[72063]
	22090.59	(0.10)	4(1, 4) - 3(1, 3)		[71046]
	22094.37	(0.10)	4(1, 4) - 3(1, 3)	1v ₃₁	[72063]
	22100.62	(0.10)	4(1, 4) - 3(1, 3)	1v ₃₂	[72063]
	22109.54	(0.10)	4(1, 4) - 3(1, 3)	2v ₃₂	[72063]
	22687.80	(0.10)	3(2, 2) - 3(1, 3)		[72063]
	22729.66	(0.10)	4(0, 4) - 3(0, 3)	4v ₃₃	[72063]
	22783.98	(0.10)	4(0, 4) - 3(0, 3)	3v ₃₃	[72063]
	22832.14	(0.10)	4(0, 4) - 3(0, 3)	2v ₃₃	[72063]
	22833.98	(0.10)	3(1, 3) - 2(0, 2)		[72063]
	22878.19	(0.10)	4(0, 4) - 3(0, 3)	1v ₃₃	[72063]
	22922.71	(0.10)	4(0, 4) - 3(0, 3)		[71046]
	22927.28	(0.10)	4(0, 4) - 3(0, 3)	1v ₃₁	[72063]
	22947.37	(0.10)	4(0, 4) - 3(0, 3)	2v ₃₂	[72063]
	22986.49	(0.10)	4(2, 3) - 3(2, 2)	4v ₃₃	[72063]
	23047.62	(0.10)	4(2, 3) - 3(2, 2)	3v ₃₃	[72063]
	23101.72	(0.10)	4(2, 3) - 3(2, 2)	2v ₃₃	[72063]
	23153.42	(0.10)	4(2, 3) - 3(2, 2)	1v ₃₃	[72063]
	23202.91	(0.10)	4(2, 3) - 3(2, 2)		[71046]
	23211.09	(0.10)	4(2, 3) - 3(2, 2)	1v ₃₁	[72063]
	23216.96	(0.10)	4(2, 3) - 3(2, 2)	1v ₃₂	[72063]
	23264.59	(0.10)	4(2, 2) - 3(2, 1)	4v ₃₃	[72063]
	23333.25	(0.10)	4(2, 2) - 3(2, 1)	3v ₃₃	[72063]
	23393.83	(0.10)	4(2, 2) - 3(2, 1)	2v ₃₃	[72063]
	23451.54	(0.10)	4(2, 2) - 3(2, 1)	1v ₃₃	[72063]
	23506.62	(0.10)	4(2, 2) - 3(2, 1)		[71046]
	23518.72	(0.10)	4(2, 2) - 3(2, 1)	1v ₃₁	[72063]
	23521.72	(0.10)	4(2, 2) - 3(2, 1)	1v ₃₂	[72063]
	23536.18	(0.10)	4(2, 2) - 3(2, 1)	2v ₃₂	[72063]
	23697.42	(0.10)	13(2, 11) - 13(2, 12)		[72063]
	23737.06	(0.10)	5(0, 5) - 4(1, 4)		[72063]
	23800.19	(0.10)	4(2, 3) - 4(1, 4)		[72063]
	23997.56	(0.10)	4(1, 3) - 3(1, 2)	4v ₃₃	[72063]
	24066.42	(0.10)	4(1, 3) - 3(1, 2)	3v ₃₃	[72063]
	24126.83	(0.10)	4(1, 3) - 3(1, 2)	2v ₃₃	[72063]
	24184.01	(0.10)	4(1, 3) - 3(1, 2)	1v ₃₃	[72063]
	24199.67	(0.10)	4(1, 3) - 3(1, 2)	1v ₃₃ , 1v ₃₂	[72063]
	24238.50	(0.10)	4(1, 3) - 3(1, 2)		[71046]
	24250.05	(0.10)	4(1, 3) - 3(1, 2)	1v ₃₁	[72063]
	24256.22	(0.10)	4(1, 3) - 3(1, 2)	1v ₃₂	[72063]
	24272.94	(0.10)	4(1, 3) - 3(1, 2)	2v ₃₂	[72063]
	24449.03	(0.10)	12(2, 10) - 12(1, 11)	1v ₃₃	[72063]
	24490.71	(0.10)	12(2, 10) - 12(1, 11)		[72063]
	26371.18	(0.10)	7(1, 6) - 6(2, 5)		[72063]
	27334.00	(0.10)	5(1, 5) - 4(1, 4)	4v ₃₃	[72063]
	27397.47	(0.10)	5(1, 5) - 4(1, 4)	3v ₃₃	[72063]
	27453.88	(0.10)	5(1, 5) - 4(1, 4)	2v ₃₃	[72063]
	27508.85	(0.10)	5(1, 5) - 4(1, 4)	1v ₃₃	[72063]
	27520.04	(0.10)	5(1, 5) - 4(1, 4)	1v ₃₃ , 1v ₃₂	[72063]
	27562.11	(0.10)	5(1, 5) - 4(1, 4)		[72063]
	27566.17	(0.10)	5(1, 4) - 4(1, 4)	1v ₃₁	[72063]
	27574.39	(0.10)	5(1, 5) - 4(1, 4)	1v ₃₂	[72063]

TABLE 42.3. Microwave spectrum of 1-pentyne — Continued

C₅H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	27582.03	(0.10)	15(3,12) - 15(2,13)		[72063]
	28389.85	(0.10)	5(0, 5) - 4(0, 4)	1ν ₃₃	[72063]
	28441.98	(0.10)	5(0, 5) - 4(0, 4)		[72063]
	28457.48	(0.10)	5(0, 5) - 4(0, 4)	1ν ₃₂	[72063]
	28639.30	(0.10)	10(1, 9) - 10(0,10)		[72063]
	28839.55	(0.10)	5(2, 4) - 4(2, 3)	2ν ₃₃	[72063]
	28885.06	(0.10)	7(2, 6) - 7(1, 7)		[72063]
	28903.36	(0.10)	5(2, 4) - 4(2, 3)	1ν ₃₃	[72063]
	28964.55	(0.10)	5(2, 4) - 4(2, 3)		[71046]
	29129.40	(0.10)	5(3, 3) - 4(3, 2)		[72063]
	29152.50	(0.10)	5(3, 2) - 4(3, 1)		[72063]
	29554.87	(0.10)	5(2, 3) - 4(2, 2)		[71046]
	29571.92	(0.10)	5(2, 3) - 4(2, 2)	1ν ₃₁	[72063]
	29574.36	(0.10)	5(2, 3) - 4(2, 2)	1ν ₃₂	[72063]
	29936.83	(0.10)	5(1, 4) - 4(1, 3)	4ν ₃₃	[72063]
	30020.94	(0.10)	5(1, 4) - 4(1, 3)	3ν ₃₃	[72063]
	30095.05	(0.10)	5(1, 4) - 4(1, 3)	2ν ₃₃	[72063]
	30165.08	(0.10)	5(1, 4) - 4(1, 3)	1ν ₃₃	[72063]
	30184.44	(0.10)	5(1, 4) - 4(1, 3)	1ν ₃₃ , 1ν ₃₂	[72063]
	30231.73	(0.10)	5(1, 4) - 4(1, 3)		[72063]
	30245.30	(0.10)	5(1, 4) - 4(1, 3)	1ν ₃₁	[72063]
	30253.65	(0.10)	5(1, 4) - 4(1, 3)	1ν ₃₂	[72063]
	32736.35	(0.10)	6(1, 6) - 5(1, 5)	4ν ₃₃	[72063]
	32810.93	(0.10)	6(1, 6) - 5(1, 5)	3ν ₃₃	[72063]
	32877.51	(0.10)	6(1, 6) - 5(1, 5)	2ν ₃₃	[72063]
	32942.15	(0.10)	6(1, 6) - 5(1, 5)	1ν ₃₃	[72063]
	32955.45	(0.10)	6(1, 6) - 5(1, 5)	1ν ₃₃ , 1ν ₃₂	[72063]
	33004.94	(0.10)	6(1, 6) - 5(1, 5)		[72063]
	33009.05	(0.10)	6(1, 6) - 5(1, 5)	1ν ₃₁	[72063]
	33019.48	(0.10)	6(1, 6) - 5(1, 5)	1ν ₃₂	[72063]
	33032.26	(0.10)	6(1, 6) - 5(1, 5)	2ν ₃₂	[72063]
	33045.15	(0.10)	11(1,10) - 11(0,11)	1ν ₃₃	[72063]
	33125.78	(0.10)	11(1,10) - 11(0,11)		[72063]
	33670.19	(0.10)	6(0, 6) - 5(0, 5)	3ν ₃₃	[72063]
	33692.72	(0.10)	6(3, 3) - 6(2, 4)		[72063]
	33703.17	(0.10)	9(2, 8) - 9(1, 9)		[72063]
	33732.81	(0.10)	6(0, 6) - 5(0, 5)	2ν ₃₃	[72063]
	33793.36	(0.10)	6(0, 6) - 5(0, 5)	1ν ₃₃	[72063]
	33808.69	(0.10)	8(1, 7) - 7(2, 6)		[72063]
	33809.49	(0.10)	6(0, 6) - 5(0, 5)	1ν ₃₃ , 1ν ₃₂	[72063]
	33852.13	(0.10)	6(0, 6) - 5(0, 5)		[72063]
	33853.40	(0.10)	6(0, 6) - 5(0, 5)	1ν ₃₁	[72063]
	33869.71	(0.10)	6(0, 6) - 5(0, 5)	1ν ₃₂	[72063]
	33884.89	(0.10)	6(0, 6) - 5(0, 5)	2ν ₃₂	[72063]
	34700.28	(0.10)	6(2, 5) - 5(2, 4)		[72063]
	34711.13	(0.10)	6(2, 5) - 5(2, 4)	1ν ₃₁	[72063]
	34720.98	(0.10)	6(2, 5) - 5(2, 4)	1ν ₃₂	[72063]
	34980.96	(0.10)	6(3, 4) - 5(3, 3)		[72063]
	35042.32	(0.10)	6(3, 3) - 5(3, 2)		[72063]
	35501.43	(0.10)	15(3,13) - 14(4,10)		[72063]
	35503.53	(0.10)	6(2, 4) - 5(2, 3)	2ν ₃₃	[72063]
	35596.70	(0.10)	6(2, 4) - 5(2, 3)	1ν ₃₃	[72063]
	35617.76	(0.10)	6(2, 4) - 5(2, 3)	1ν ₃₃ , 1ν ₃₂	[72063]
	35685.33	(0.10)	6(2, 4) - 5(2, 3)		[72063]
	35707.62	(0.10)	6(2, 4) - 5(2, 3)	1ν ₃₁	[72063]
	35709.52	(0.10)	6(2, 4) - 5(2, 3)	1ν ₃₂	[72063]
	36174.52	(0.10)	6(1, 5) - 5(1, 4)		[72063]
	36189.16	(0.10)	6(1, 5) - 5(1, 4)	1ν ₃₁	[72063]
	36200.48	(0.10)	6(1, 5) - 5(1, 4)	1ν ₃₂	[72063]
<i>t</i> -H ₃ CH ₂ CH ₂ CCH	8579.72	(0.10)	2(1, 2) - 1(1, 1)		[72063]
	8693.36	(0.10)	2(0, 2) - 1(0, 1)		[71046]
	8705.28	(0.10)	2(0, 2) - 1(0, 1)	1ν ₃₃	[72063]
	8808.11	(0.10)	2(1, 1) - 1(1, 0)		[72063]
	12859.73	(0.10)	3(1, 3) - 2(1, 2)	1ν ₃₁	[72063]
	12869.32	(0.10)	3(1, 3) - 2(1, 2)		[71046]
	12881.82	(0.10)	3(1, 3) - 2(1, 2)	1ν ₃₃ , 1ν ₃₁	[72063]
	12885.50	(0.10)	3(1, 3) - 2(1, 2)	1ν ₃₂	[72063]

TABLE 42.3. Microwave spectrum of 1-pentyne — Continued

C₅H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	12892.30	(0.10)	3(1, 3) - 2(1, 2)	1ν ₃₃	[72063]
	12908.13	(0.10)	3(1, 3) - 2(1, 2)	1ν ₃₃ , 1ν ₃₂	[72063]
	12916.15	(0.10)	3(1, 3) - 2(1, 2)	2ν ₃₃	[72063]
	12941.07	(0.10)	3(1, 3) - 2(1, 2)	3ν ₃₃	[72063]
	13028.38	(0.10)	3(0, 3) - 2(0, 2)	1ν ₃₁	[72063]
	13038.87	(0.10)	3(0, 3) - 2(0, 2)		[72063]
	13056.68	(0.10)	3(0, 3) - 2(0, 2)	1ν ₃₃	[72063]
	13059.81	(0.10)	3(0, 3) - 2(0, 2)	1ν ₃₂	[72063]
	13211.74	(0.10)	3(1, 2) - 2(1, 1)		[71046]
	13224.27	(0.10)	3(1, 2) - 2(1, 1)	1ν ₃₃	[72063]
	13237.56	(0.20)	3(1, 2) - 2(1, 1)	2ν ₃₃	[72063]
	13237.56	(0.20)	3(1, 2) - 2(1, 1)	1ν ₃₂	[72063]
	17145.89	(0.10)	4(1, 4) - 3(1, 3)	1ν ₃₁	[72063]
	17158.42	(0.10)	4(1, 4) - 3(1, 3)		[71046]
	17180.08	(0.10)	4(1, 4) - 3(1, 3)	1ν ₃₂	[72063]
	17189.12	(0.10)	4(1, 4) - 3(1, 3)	1ν ₃₃	[72063]
	17210.25	(0.10)	4(1, 4) - 3(1, 3)	1ν ₃₃ , 1ν ₃₂	[72063]
	17221.07	(0.10)	4(1, 4) - 3(1, 3)	2ν ₃₃	[72063]
	17254.19	(0.10)	4(1, 4) - 3(1, 3)	3ν ₃₃	[72063]
	17288.90	(0.10)	4(1, 4) - 3(1, 3)	4ν ₃₃	[72063]
	17383.10	(0.10)	4(0, 4) - 3(0, 3)		[71046]
	17599.48	(0.10)	4(1, 3) - 3(1, 2)	1ν ₃₁	[72063]
	17615.27	(0.10)	4(1, 3) - 3(1, 2)		[71046]
	17631.78	(0.10)	4(1, 3) - 3(1, 2)	1ν ₃₃	[72063]
	17649.58	(0.20)	4(1, 3) - 3(1, 2)	2ν ₃₃	[72063]
	17649.58	(0.20)	4(1, 3) - 3(1, 2)	1ν ₃₂	[72063]
	17663.34	(0.10)	4(1, 3) - 3(1, 2)	1ν ₃₃ , 1ν ₃₂	[72063]
	17668.98	(0.10)	4(1, 3) - 3(1, 2)	3ν ₃₃	[72063]
	21431.54	(0.10)	5(1, 5) - 4(1, 4)	1ν ₃₁	[72063]
	21447.14	(0.10)	5(1, 5) - 4(1, 4)		[71046]
	21467.91	(0.10)	5(1, 5) - 4(1, 4)	1ν ₃₃ , 1ν ₃₁	[72063]
	21474.26	(0.10)	5(1, 5) - 4(1, 4)	1ν ₃₂	[72063]
	21485.44	(0.10)	5(1, 5) - 4(1, 4)	1ν ₃₃	[72063]
	21500.25	(0.10)	5(1, 5) - 4(1, 4)	2ν ₃₂	[72063]
	21511.90	(0.10)	5(1, 5) - 4(1, 4)	1ν ₃₃ , 1ν ₃₂	[72063]
	21525.47	(0.10)	5(1, 5) - 4(1, 4)	2ν ₃₃	[72063]
	21566.96	(0.10)	5(1, 5) - 4(1, 4)	3ν ₃₃	[72063]
	21610.32	(0.10)	5(1, 5) - 4(1, 4)	4ν ₃₃	[72063]
	21707.80	(0.10)	5(0, 5) - 4(0, 4)	1ν ₃₁	[72063]
	21725.31	(0.10)	5(0, 5) - 4(0, 4)		[71046]
	21734.04	(0.10)	5(2, 4) - 4(2, 3)		[71046]
	21743.17	(0.10)	5(2, 3) - 4(2, 2)		[71046]
	21755.04	(0.10)	5(0, 5) - 4(0, 4)	1ν ₃₃	[72063]
	21760.17	(0.10)	5(0, 5) - 4(0, 4)	1ν ₃₂	[72063]
	21772.25	(0.10)	5(2, 3) - 4(2, 2)	1ν ₃₃	[72063]
	21786.41	(0.10)	5(0, 5) - 4(0, 4)	2ν ₃₃	[72063]
	21787.84	(0.10)	5(0, 5) - 4(0, 4)	1ν ₃₃ , 1ν ₃₂	[72063]
	21854.28	(0.10)	5(0, 5) - 4(0, 4)	4ν ₃₃	[72063]
	21998.45	(0.10)	5(1, 4) - 4(1, 3)	1ν ₃₁	[72063]
	22018.18	(0.10)	5(1, 4) - 4(1, 3)		[71046]
	22038.86	(0.10)	5(1, 4) - 4(1, 3)	1ν ₃₂	[72063]
	22061.06	(0.30)	5(1, 4) - 4(1, 3)	2ν ₃₃	[72063]
	22061.06	(0.30)	5(1, 4) - 4(1, 3)	1ν ₃₂	[72063]
	22078.27	(0.10)	5(1, 4) - 4(1, 3)	1ν ₃₃ , 1ν ₃₂	[72063]
	22085.37	(0.10)	5(1, 4) - 4(1, 3)	3ν ₃₃	[72063]
	22102.49	(0.10)	5(1, 4) - 4(1, 3)	2ν ₃₂	[72063]
	22111.18	(0.10)	5(1, 4) - 4(1, 3)	4ν ₃₃	[72063]
	25716.40	(0.10)	6(1, 6) - 5(1, 5)	1ν ₃₁	[72063]
	25735.28	(0.10)	6(1, 6) - 5(1, 5)		[71046]
	25767.65	(0.10)	6(1, 6) - 5(1, 5)	1ν ₃₂	[72063]
	25781.29	(0.10)	6(1, 6) - 5(1, 5)	1ν ₃₃	[72063]
	25798.99	(0.10)	6(1, 6) - 5(1, 5)	2ν ₃₂	[72063]
	25813.03	(0.10)	6(1, 6) - 5(1, 5)	1ν ₃₃ , 1ν ₃₂	[72063]
	25829.30	(0.10)	6(1, 6) - 5(1, 5)	2ν ₃₃	[72063]
	25879.03	(0.10)	6(1, 6) - 5(1, 5)	3ν ₃₃	[72063]
	25931.16	(0.10)	6(1, 6) - 5(1, 5)	4ν ₃₃	[72063]
	26044.24	(0.10)	6(0, 6) - 5(0, 5)	1ν ₃₁	[72063]

TABLE 42.3. Microwave spectrum of 1-pentyne — Continued

C₅H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	26065.28	(0.10)	6(0, 6) - 5(0, 5)		[71046]
	26079.88	(0.10)	6(2, 5) - 5(2, 4)		[71046]
	26095.81	(0.10)	6(2, 4) - 5(2, 3)		[71046]
	26100.92	(0.10)	6(0, 6) - 5(0, 5)	1ν ₃₃	[72063]
	26106.86	(0.10)	6(0, 6) - 5(0, 5)	1ν ₃₂	[72063]
	26138.20	(0.10)	6(2, 4) - 5(2, 3)	1ν ₃₂	[72063]
	26138.66	(0.10)	6(0, 6) - 5(0, 5)	2ν ₃₃	[72063]
	26140.20	(0.10)	6(0, 6) - 5(0, 5)	1ν ₃₃ , 1ν ₃₂	[72063]
	26220.60	(0.10)	6(0, 6) - 5(0, 5)	4ν ₃₃	[72063]
	26396.80	(0.10)	6(1, 5) - 5(1, 4)	1ν ₃₁	[72063]
	26420.37	(0.10)	6(1, 5) - 5(1, 4)		[71046]
	26423.03	(0.10)	6(1, 5) - 5(1, 4)	1ν ₃₃ 1ν ₃₁	[72063]
	26445.27	(0.10)	6(1, 5) - 5(1, 4)	1ν ₃₃	[72063]
	26471.77	(0.20)	6(1, 5) - 5(1, 4)	1ν ₃₂	[72063]
	26472.12	(0.20)	6(1, 5) - 5(1, 4)	2ν ₃₃	[72063]
	26492.48	(0.10)	6(1, 5) - 5(1, 4)	1ν ₃₃ , 1ν ₃₂	[72063]
	26501.10	(0.10)	6(1, 5) - 5(1, 4)	3ν ₃₃	[72063]
	26521.54	(0.10)	6(1, 5) - 5(1, 4)	2ν ₃₂	[72063]
	26532.18	(0.10)	6(1, 5) - 5(1, 4)	4ν ₃₃	[72063]
	30000.76	(0.10)	7(1, 7) - 6(1, 6)	1ν ₃₁	[72063]
	30022.62	(0.10)	7(1, 7) - 6(1, 6)		[71046]
	30060.35	(0.10)	7(1, 7) - 6(1, 6)	1ν ₃₂	[72063]
	30076.42	(0.10)	7(1, 7) - 6(1, 6)	1ν ₃₃	[72063]
	30113.33	(0.10)	7(1, 7) - 6(1, 6)	1ν ₃₃ , 1ν ₃₂	[72063]
	30132.29	(0.10)	7(1, 7) - 6(1, 6)	2ν ₃₃	[72063]
	30190.47	(0.10)	7(1, 7) - 6(1, 6)	3ν ₃₃	[72063]
	30402.31	(0.10)	7(0, 7) - 6(0, 6)		[72063]
	30425.23	(0.10)	7(2, 6) - 6(2, 5)		[71046]
	30450.98	(0.10)	7(2, 5) - 6(2, 4)		[71046]
	30466.57	(0.10)	7(2, 6) - 6(2, 5)	1ν ₃₃	[72063]
	30474.47	(0.10)	7(2, 6) - 6(2, 5)	1ν ₃₂	[72063]
	30794.40	(0.10)	7(1, 6) - 6(1, 5)	1ν ₃₁	[72063]
	30821.85	(0.10)	7(1, 6) - 6(1, 5)		[71046]
	30825.02	(0.10)	7(1, 6) - 6(1, 5)	1ν ₃₃ , 1ν ₃₁	[72063]
	30850.93	(0.10)	7(1, 6) - 6(1, 5)	1ν ₃₃	[72063]
	30881.76	(0.10)	7(1, 6) - 6(1, 5)	1ν ₃₂	[72063]
	30882.32	(0.10)	7(1, 6) - 6(1, 5)	2ν ₃₃	[72063]
	30905.99	(0.10)	7(1, 6) - 6(1, 5)	1ν ₃₃ , 1ν ₃₂	[72063]
	30916.22	(0.10)	7(1, 6) - 6(1, 5)	3ν ₃₃	[72063]
	30952.40	(0.10)	7(1, 6) - 6(1, 5)	4ν ₃₃	[72063]
	34284.14	(0.10)	8(1, 8) - 7(1, 7)	1ν ₃₁	[72063]
	34309.15	(0.10)	8(1, 8) - 7(1, 7)		[71046]
	34352.21	(0.10)	8(1, 8) - 7(1, 7)	1ν ₃₂	[72063]
	34370.65	(0.10)	8(1, 8) - 7(1, 7)	1ν ₃₃	[72063]
	34412.82	(0.10)	8(1, 8) - 7(1, 7)	1ν ₃₃ , 1ν ₃₂	[72063]
	34434.62	(0.10)	8(1, 8) - 7(1, 7)	2ν ₃₃	[72063]
	34501.17	(0.10)	8(1, 8) - 7(1, 7)	3ν ₃₃	[72063]
	34570.85	(0.10)	8(1, 8) - 7(1, 7)	4ν ₃₃	[72063]
	34736.11	(0.10)	8(0, 8) - 7(0, 7)		[72063]
	34769.94	(0.10)	8(2, 7) - 7(2, 6)		[71046]
	34808.59	(0.10)	8(2, 6) - 7(2, 5)		[71046]
	34817.26	(0.10)	8(2, 7) - 7(2, 6)	1ν ₃₃	[72063]
	35191.08	(0.10)	8(1, 7) - 7(1, 6)	1ν ₃₁	[72063]
	35222.36	(0.10)	8(1, 7) - 7(1, 6)		[71046]
	35255.63	(0.10)	8(1, 7) - 7(1, 6)	1ν ₃₃	[72063]
	35290.81	(0.10)	8(1, 7) - 7(1, 6)	1ν ₃₂	[72063]
	35291.63	(0.10)	8(1, 7) - 7(1, 6)	2ν ₃₃	[72063]
	35318.57	(0.10)	8(1, 7) - 7(1, 6)	1ν ₃₃ , 1ν ₃₂	[72063]
	35330.37	(0.10)	8(1, 7) - 7(1, 6)	3ν ₃₃	[72063]
	35371.72	(0.10)	8(1, 7) - 7(1, 6)	4ν ₃₃	[72063]
	39066.24	(0.10)	9(0, 9) - 8(0, 8)		[72063]
	39113.97	(0.10)	9(2, 8) - 8(2, 7)		[72063]
	39659.38	(0.10)	9(1, 8) - 8(1, 7)	1ν ₃₃	[72063]

Table 43.1. Molecular constants of trans-vinyl cyclopropane.

Species	v	A (MHz)	B (MHz)	C (MHz)	Reference
$\text{CH}(\text{CHCH}_2)\text{CH}_2\text{CH}_2$	0	15262.(79) ^a	3061.368(19)	2941.132(18)	[present]
	1	15092.(150)	3071.43(5)	2944.02(5)	[74063]
	2	14794.(150)	3081.38(5)	2946.70(5)	[74063]
	3	14875.(150)	3091.22(5)	2949.27(5)	[74063]
$\text{CH}(\text{CHCH}_2)^{13}\text{CH}_2\text{CH}_2$	0	15067. ^b	3022.66(10)	2896.45(10)	[74063]
<u>Electric Dipole Moments for $\text{CH}(\text{CHCH}_2)\text{CH}_2\text{CH}_2$ [74063]</u>					
μ_a		0.486(7) D			
μ_c		0.110(10) D			

^aThe numbers in parentheses represent one standard deviation of the fit.

^bAssumed value.

TABLE 43.2. Microwave spectrum of vinylcyclopropane

C₃H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
$t\text{-CH}(\text{CHCH}_2)\text{CH}_2\text{CH}_2$	11885.44	(0.05)	2(1, 2) - 1(1, 1)		[74063]
	12004.64	(0.05)	2(0, 2) - 1(0, 1)		[74063]
	12125.54	(0.05)	2(1, 1) - 1(1, 0)		[74063]
	17827.57	(0.05)	3(1, 3) - 2(1, 2)		[74063]
$\begin{array}{c} \text{H}_2\text{C}-\text{CH}_2 \\ \diagdown \\ \text{CH} \\ \\ \text{CH} \\ \\ \text{CH}_2 \end{array}$	18004.72	(0.05)	3(0, 3) - 2(0, 2)		[74063]
	23768.99	(0.05)	4(1, 4) - 3(1, 3)		[74063]
	24002.00	(0.05)	4(0, 4) - 3(0, 3)		[74063]
	24010.01	(0.05)	4(2, 3) - 3(2, 2)		[74063]
	24012.07	(0.05)	4(3, 1) - 3(3, 0)		[74063]
	24018.91	(0.05)	4(2, 2) - 3(2, 1)		[74063]
	24249.20	(0.05)	4(1, 3) - 3(1, 2)		[74063]
	29709.50	(0.05)	5(1, 5) - 4(1, 4)		[74063]
	29995.72	(0.05)	5(0, 5) - 4(0, 4)		[74063]
	30011.29	(0.05)	5(2, 4) - 4(2, 3)		[74063]
	30029.12	(0.05)	5(2, 3) - 4(2, 2)		[74063]
	30309.71	(0.05)	5(1, 4) - 4(1, 3)		[74063]
	11903.60	(0.05)	2(1, 2) - 1(1, 1)	1 ν_{33}	[74063]
	12029.99	(0.05)	2(0, 2) - 1(0, 1)	1 ν_{33}	[74063]
	12158.41	(0.05)	2(1, 1) - 1(1, 0)	1 ν_{33}	[74063]
	24053.84	(0.05)	4(0, 4) - 3(0, 3)	1 ν_{33}	[74063]
	24060.90	(0.05)	4(2, 3) - 3(2, 2)	1 ν_{33}	[74063]
	29754.32	(0.05)	5(1, 5) - 4(1, 4)	1 ν_{33}	[74063]
	30057.05	(0.05)	5(0, 5) - 4(0, 4)	1 ν_{33}	[74063]
	30074.74	(0.05)	5(2, 4) - 4(2, 3)	1 ν_{33}	[74063]
	30095.08	(0.05)	5(2, 3) - 4(2, 2)	1 ν_{33}	[74063]
	30391.32	(0.05)	5(1, 4) - 4(1, 3)	1 ν_{33}	[74063]
	23840.84	(0.05)	4(1, 4) - 3(1, 3)	2 ν_{33}	[74063]
	29798.84	(0.05)	5(1, 5) - 4(1, 4)	2 ν_{33}	[74063]
	30117.72	(0.05)	5(0, 5) - 4(0, 4)	2 ν_{33}	[74063]
	30137.72	(0.05)	5(2, 4) - 4(2, 3)	2 ν_{33}	[74063]
	30160.66	(0.05)	5(2, 3) - 4(2, 3)	2 ν_{33}	[74063]
30472.21	(0.05)	5(1, 4) - 4(1, 3)	2 ν_{33}	[74063]	
29842.29	(0.05)	5(1, 5) - 4(1, 4)	3 ν_{33}	[74063]	
30177.06	(0.05)	5(0, 5) - 4(0, 4)	3 ν_{33}	[74063]	
30199.51	(0.05)	5(2, 4) - 4(2, 3)	3 ν_{33}	[74063]	
30225.19	(0.05)	5(2, 3) - 4(2, 2)	3 ν_{33}	[74063]	
$t\text{-CH}(\text{CHCH}_2)^{13}\text{CH}_2\text{CH}_2$	23666.5	(0.15)	4(0, 4) - 3(0, 3)		[74063]
	23927.0	(0.2)	4(1, 3) - 3(1, 2)		[74063]
	29275.9	(0.2)	5(1, 5) - 4(1, 4)		[74063]
	29575.7	(0.2)	5(0, 5) - 4(0, 4)		[74063]
	29593.1	(0.2)	5(2, 4) - 4(2, 3)		[74063]
	29906.8	(0.2)	5(1, 4) - 4(1, 3)		[74063]

Table 44.1. Molecular constants for methylene cyclobutane.

Vibrational State ^a	v	A (MHz)	B (MHz)	C (MHz)
<u>CH₂CCH₂CH₂CH₂</u>				
<u>Rotational Constants [68044]</u>				
	0	10373.9(16)	4618.05(6)	3459.87(5)
	1	10368.8(16)	4592.21(6)	3462.95(5)
	2	10434.9(20)	4587.03(10)	3431.93(10)
	3	10358.9(20)	4603.81(10)	3460.43(10)
	4	10357.9(20)	4603.03(10)	3458.40(10)
	5	10308.6(20)	4613.34(10)	3475.42(10)
	6	10276.3(20)	4619.52(10)	3465.22(10)
<u>Zeeman Constants v=2 State [70063]</u>				
g_{aa}		-0.0320(8)	μ_N	
g_{bb}		-0.0218(10)	μ_N	
g_{cc}		-0.0184(11)	μ_N	
$2\chi_{aa}-\chi_{bb}-\chi_{cc}$		-6.4(5)	$10^{-6} \text{erg}/(\text{G}^2 \cdot \text{mol})$	
$-\chi_{aa}+2\chi_{bb}-\chi_{cc}$		4.3(17)	$10^{-6} \text{erg}/(\text{G}^2 \cdot \text{mol})$	
Q_{aa}		-1.2(11)	$10^{-26} \text{esu} \cdot \text{cm}^2$	
Q_{bb}		-1.1(20)	$10^{-26} \text{esu} \cdot \text{cm}^2$	
Q_{cc}		2.3(24)	$10^{-26} \text{esu} \cdot \text{cm}^2$	

^aRing puckering vibration.

TABLE 44.2. Microwave spectrum of methylene cyclobutane

C₃H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
CH ₂ CCH ₂ CH ₂ CH ₂	8019.04	(0.05)	1(0, 1) - 0(0, 0)	2ν _p	[68044]
	8061.43	(0.05)	1(0, 1) - 0(0, 0)	4ν _p	[68044]
	8064.21	(0.05)	1(0, 1) - 0(0, 0)	3ν _p	[68044]
$\begin{array}{c} \text{H}_2\text{C}-\text{C}=\text{CH}_2 \\ \quad \\ \text{H}_2\text{C}-\text{CH}_2 \end{array}$	8066.56	(0.05)	1(0, 1) - 0(0, 0)	[68044]	[68044]
	8072.57	(0.05)	1(0, 1) - 0(0, 0)	1ν _p	[68044]
	8088.74	(0.05)	1(0, 1) - 0(0, 0)	5ν _p	[68044]
	8104.74	(0.05)	1(0, 1) - 0(0, 0)	6ν _p	[68044]
	14882.80	(0.05)	2(1, 2) - 1(1, 1)	2ν _p	[68044]
	14978.21	(0.05)	2(1, 2) - 1(1, 1)	4ν _p	[68044]
	14985.08	(0.05)	2(1, 2) - 1(1, 1)	3ν _p	[68044]
	14989.22	(0.05)	2(1, 2) - 1(1, 1)	[68044]	[68044]
	15017.02	(0.05)	2(1, 2) - 1(1, 1)	1ν _p	[68044]
	15039.60	(0.05)	2(1, 2) - 1(1, 1)	5ν _p	[68044]
	15075.19	(0.05)	2(1, 2) - 1(1, 1)	6ν _p	[68044]
	15883.156	(0.003)	2(0, 2) - 1(0, 1)	2ν _p	[70063]
	15968.47	(0.05)	2(0, 2) - 1(0, 1)	4ν _p	[68044]
	15974.41	(0.05)	2(0, 2) - 1(0, 1)	3ν _p	[68044]
	15979.45	(0.05)	2(0, 2) - 1(0, 1)	[68044]	[68044]
	15992.70	(0.05)	2(0, 2) - 1(0, 1)	1ν _p	[68044]
	16023.42	(0.05)	2(0, 2) - 1(0, 1)	5ν _p	[68044]
	16055.40	(0.05)	2(0, 2) - 1(0, 1)	6ν _p	[68044]
	17193.087	(0.030)	2(1, 1) - 1(1, 0)	2ν _p	[70063]
	17267.47	(0.05)	2(1, 1) - 1(1, 0)	4ν _p	[68044]
	17270.27	(0.05)	2(1, 1) - 1(1, 0)	[68044]	[68044]
	17271.84	(0.05)	2(1, 1) - 1(1, 0)	3ν _p	[68044]
	17295.12	(0.05)	2(1, 1) - 1(1, 0)	1ν _p	[68044]
	17315.45	(0.05)	2(1, 1) - 1(1, 0)	5ν _p	[68044]
	17343.79	(0.05)	2(1, 1) - 1(1, 0)	6ν _p	[68044]
	22233.08	(0.05)	3(1, 3) - 2(1, 2)	2ν _p	[68044]
	22376.57	(0.05)	3(1, 3) - 2(1, 2)	4ν _p	[68044]
	22387.13	(0.05)	3(1, 3) - 2(1, 2)	3ν _p	[68044]
	22393.03	(0.05)	3(1, 3) - 2(1, 2)	[68044]	[68044]
	22444.99	(0.05)	3(1, 3) - 2(1, 2)	1ν _p	[68044]
	22468.85	(0.05)	3(1, 3) - 2(1, 2)	5ν _p	[68044]
	22522.22	(0.05)	3(1, 3) - 2(1, 2)	6ν _p	[68044]
	23454.99	(0.05)	3(0, 3) - 2(0, 2)	2ν _p	[68044]
	23584.47	(0.05)	3(0, 3) - 2(0, 2)	4ν _p	[68044]
	23594.34	(0.05)	3(0, 3) - 2(0, 2)	3ν _p	[68044]
	23602.37	(0.05)	3(0, 3) - 2(0, 2)	[68044]	[68044]
23625.70	(0.05)	3(0, 3) - 2(0, 2)	1ν _p	[68044]	
23667.75	(0.05)	3(0, 3) - 2(0, 2)	5ν _p	[68044]	
23715.78	(0.05)	3(0, 3) - 2(0, 2)	6ν _p	[68044]	
24056.33	(0.01)	3(2, 2) - 2(1, 1)	2ν _p	[70063]	
24160.30	(0.05)	3(2, 2) - 2(1, 1)	[68044]	[68044]	
24184.17	(0.05)	3(2, 2) - 2(1, 1)	4ν _p	[68044]	
24193.10	(0.05)	3(2, 2) - 2(1, 1)	3ν _p	[68044]	
24266.17	(0.05)	3(2, 2) - 2(1, 1)	5ν _p	[68044]	
24314.17	(0.05)	3(2, 2) - 2(1, 1)	6ν _p	[68044]	
24541.66	(0.05)	3(2, 2) - 2(1, 1)	1ν _p	[68044]	
24658.24	(0.05)	3(2, 1) - 2(2, 0)	2ν _p	[68044]	
24772.49	(0.05)	3(2, 1) - 2(2, 0)	[68044]	[68044]	
24783.84	(0.05)	3(2, 1) - 2(2, 0)	4ν _p	[68044]	
24791.26	(0.05)	3(2, 1) - 2(2, 0)	3ν _p	[68044]	
24864.70	(0.05)	3(2, 1) - 2(2, 0)	5ν _p	[68044]	
24912.55	(0.05)	3(2, 1) - 2(2, 0)	6ν _p	[68044]	
25053.92	(0.05)	3(2, 1) - 2(2, 0)	1ν _p	[68044]	
25685.32	(0.05)	3(1, 2) - 2(1, 1)	2ν _p	[68044]	
25797.25	(0.05)	3(1, 2) - 2(1, 1)	4ν _p	[68044]	
25799.33	(0.05)	3(1, 2) - 2(1, 1)	[68044]	[68044]	
25804.16	(0.05)	3(1, 2) - 2(1, 1)	3ν _p	[68044]	
25839.36	(0.05)	3(1, 2) - 2(1, 1)	1ν _p	[68044]	
25869.38	(0.05)	3(1, 2) - 2(1, 1)	5ν _p	[68044]	
25911.91	(0.05)	3(1, 2) - 2(1, 1)	6ν _p	[68044]	
29491.03	(0.05)	4(1, 4) - 3(1, 3)	2ν _p	[68044]	
29683.15	(0.05)	4(1, 4) - 3(1, 3)	4ν _p	[68044]	
29697.62	(0.05)	4(1, 4) - 3(1, 3)	3ν _p	[68044]	
29705.05	(0.05)	4(1, 4) - 3(1, 3)	[68044]	[68044]	

TABLE 44.2. Microwave spectrum of methylene cyclobutane — Continued

C₃H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	29803.94	(0.05)	4(1, 4) - 3(1, 3)	1 ν_p	[68044]
	29806.53	(0.05)	4(1, 4) - 3(1, 3)	5 ν_p	[68044]
	29877.75	(0.05)	4(1, 4) - 3(1, 3)	6 ν_p	[68044]
	30669.83	(0.05)	4(0, 4) - 3(0, 3)	2 ν_p	[68044]
	30870.65	(0.05)	4(0, 4) - 3(0, 3)		[68044]
	30845.70	(0.05)	4(0, 4) - 3(0, 3)	4 ν_p	[68044]
	30860.24	(0.05)	4(0, 4) - 3(0, 3)	3 ν_p	[68044]
	30910.21	(0.05)	4(0, 4) - 3(0, 3)	1 ν_p	[68044]
	30958.68	(0.05)	4(0, 4) - 3(0, 3)	5 ν_p	[68044]
	31023.29	(0.05)	4(0, 4) - 3(0, 3)	6 ν_p	[68044]
	31953.83	(0.05)	4(2, 3) - 3(2, 2)	2 ν_p	[68044]
	32064.71	(0.05)	4(2, 3) - 3(2, 2)		[68044]
	32092.58	(0.05)	4(3, 2) - 3(3, 1)		[68044]
	32124.78	(0.05)	4(2, 3) - 3(2, 2)	4 ν_p	[68044]
	32137.13	(0.05)	4(2, 3) - 3(2, 2)	3 ν_p	[68044]
	32234.43	(0.05)	4(2, 3) - 3(2, 2)	5 ν_p	[68044]
	32298.35	(0.05)	4(2, 3) - 3(2, 2)	6 ν_p	[68044]
	32348.07	(0.05)	4(3, 2) - 3(3, 1)	2 ν_p	[68044]
	32407.05	(0.05)	4(3, 2) - 3(3, 1)	1 ν_p	[68044]
	32425.86	(0.05)	4(3, 1) - 3(3, 0)	2 ν_p	[68044]
	32445.01	(0.05)	4(3, 1) - 3(3, 0)		[68044]
	32482.60	(0.05)	4(3, 1) - 3(3, 0)	1 ν_p	[68044]
	32518.37	(0.05)	4(3, 2) - 3(3, 1)	4 ν_p	[68044]
	32530.78	(0.05)	4(3, 2) - 3(3, 1)	3 ν_p	[68044]
	32596.27	(0.05)	4(3, 1) - 3(3, 0)	4 ν_p	[68044]
	32608.25	(0.05)	4(3, 1) - 3(3, 0)	3 ν_p	[68044]
	32627.44	(0.05)	4(3, 2) - 3(3, 1)	5 ν_p	[68044]
	32691.23	(0.05)	4(3, 2) - 3(3, 1)	6 ν_p	[68044]
	32705.46	(0.05)	4(3, 1) - 3(3, 0)	5 ν_p	[68044]
	32769.54	(0.05)	4(3, 1) - 3(3, 0)	6 ν_p	[68044]
	33359.01	(0.05)	4(2, 2) - 3(2, 1)	2 ν_p	[68044]
	33523.72	(0.05)	4(2, 2) - 3(2, 1)	4 ν_p	[68044]
	33506.17	(0.05)	4(2, 2) - 3(2, 1)		[68044]
	33532.58	(0.05)	4(2, 2) - 3(2, 1)	3 ν_p	[68044]
	33599.42	(0.05)	4(2, 3) - 3(2, 2)	1 ν_p	[68044]
	33629.78	(0.05)	4(2, 2) - 3(2, 1)	5 ν_p	[68044]
	33693.03	(0.05)	4(2, 2) - 3(2, 1)	6 ν_p	[68044]
	33714.43	(0.05)	4(2, 2) - 3(2, 1)	1 ν_p	[68044]
	34033.71	(0.05)	4(1, 3) - 3(1, 2)	2 ν_p	[68044]
	34179.86	(0.05)	4(1, 3) - 3(1, 2)		[68044]
	34183.52	(0.05)	4(1, 3) - 3(1, 2)	4 ν_p	[68044]
	34193.42	(0.05)	4(1, 3) - 3(1, 2)	3 ν_p	[68044]
	34243.14	(0.05)	4(1, 3) - 3(1, 2)	1 ν_p	[68044]
	34279.98	(0.05)	4(1, 3) - 3(1, 2)	5 ν_p	[68044]
	34336.55	(0.05)	4(1, 3) - 3(1, 2)	6 ν_p	[68044]
	36651.14	(0.05)	5(1, 5) - 4(1, 4)	2 ν_p	[68044]
	36892.54	(0.05)	5(1, 5) - 4(1, 4)	4 ν_p	[68044]
	36911.07	(0.05)	5(1, 5) - 4(1, 4)	3 ν_p	[68044]
	36919.56	(0.05)	5(1, 5) - 4(1, 4)		[68044]
	37047.41	(0.05)	5(1, 5) - 4(1, 4)	5 ν_p	[68044]
	37136.64	(0.05)	5(1, 5) - 4(1, 4)	6 ν_p	[68044]
	37141.00	(0.05)	5(1, 5) - 4(1, 4)	1 ν_p	[68044]
	37590.34	(0.05)	5(0, 5) - 4(0, 4)	2 ν_p	[68044]
	37815.95	(0.05)	5(0, 5) - 4(0, 4)	4 ν_p	[68044]
	37835.34	(0.05)	5(0, 5) - 4(0, 4)	3 ν_p	[68044]
	37846.63	(0.05)	5(0, 5) - 4(0, 4)		[68044]
	37920.11	(0.05)	5(0, 5) - 4(0, 4)	1 ν_p	[68044]
	37960.66	(0.05)	5(0, 5) - 4(0, 4)	5 ν_p	[68044]
	38043.16	(0.05)	5(0, 5) - 4(0, 4)	6 ν_p	[68044]
	39749.52	(0.05)	5(2, 4) - 4(2, 3)	2 ν_p	[68044]
	39792.83	(0.05)	5(2, 4) - 4(2, 3)		[68044]
	39964.04	(0.05)	5(2, 4) - 4(2, 3)	4 ν_p	[68044]
	39980.24	(0.05)	5(2, 4) - 4(2, 3)	3 ν_p	[68044]
	40086.12	(0.05)	5(3, 3) - 4(3, 2)		[68044]
	40571.01	(0.05)	5(4, 2) - 4(4, 1)	1 ν_p	[68044]
	40572.65	(0.05)	5(3, 3) - 4(3, 2)	1 ν_p	[68044]
	40577.72	(0.05)	5(4, 1) - 4(4, 0)	1 ν_p	[68044]

TABLE 44.2. Microwave spectrum of methylene cyclobutane — Continued

C₄H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	40654.28	(0.05)	5(2, 4) - 4(2, 3)	1ν _p	[68044]
	40827.63	(0.05)	5(3, 2) - 4(3, 1)	1ν _p	[68044]
	40844.02	(0.05)	5(4, 2) - 4(4, 1)		[68044]
	40858.29	(0.05)	5(4, 1) - 4(4, 0)		[68044]
	40909.99	(0.05)	5(3, 2) - 4(3, 1)		[68044]
	42324.34	(0.05)	5(1, 4) - 4(1, 3)		[68044]
	42420.05	(0.05)	5(2, 3) - 4(2, 2)		[68044]
	42433.65	(0.05)	5(1, 4) - 4(1, 3)	1ν _p	[68044]
	42564.68	(0.05)	5(2, 3) - 4(2, 2)	1ν _p	[68044]

Table 45.1. Molecular constants for 1-methyl cyclobutene.

Parameter	CH ₃ -C=CHCH ₂ CH ₂	CH ₃ -C=CHCH ₂ CH ₂
	Ground State [present]	Torsional Excited State [70069]
A (MHz)	11679.182(23)	11653.63
B (MHz)	4219.51(10)	4214.93
C (MHz)	3292.015(8)	3290.19
Δ _J (MHz)	1.02(21)	
Δ _{JK} (kHz)	3.49(65)	
Δ _K (kHz)	-12.9(57)	
δ _J (kHz)	0.068(29)	
δ _K (kHz)	3.73(87)	
<u>Internal Rotation Constants</u>		
I _α (u Å ²)	3.16 ^a	3.13 ^a
λ _a	0.9945	0.9945
λ _b	0.1045	0.1045
θ	6.0° ^a	---
s	43.63	44.33
F (GHz)	172.43	175.04
V ₃ (cm ⁻¹)	565.1(7)	583.(4)
V ₆ (cm ⁻¹)	---	-13.7(88)
<u>Electric Dipole Moment</u> [70069]		
μ _a (D)	0.322(10)	
μ _b (D)	0.156(12)	

^aAssumed value.

Comments: Several errors in reference [70069] have been corrected. The 2₁₁-2₀₂ transition frequency should be 9395.59, and the A,E assignments of the 3₁₂-3₀₃ transition are reversed. The quantum numbers for the transition at 22213.7 MHz should be 3₀₃ (not 2₀₃) and the line at 30222. MHz should be 3₃₀ (not 3₀₃). The 5₂₄-5₁₅ E transition at 30990.92 deviates by 1 MHz and was not fit.

TABLE 45.2. Microwave spectrum of 1-methylcyclobutene

C₅H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_1	Sym.	Ref.
C(CH ₃)CHCH ₂ CH ₂	9395.59	(0.10)	2(1, 1) - 2(0, 2)		E	[70069]
	9396.49	(0.10)	2(1, 1) - 2(0, 2)		A	[70069]
$\begin{array}{c} \text{H}_2\text{C}-\text{CH}_2 \\ \quad \\ \text{HC}=\text{C}-\text{CH}_3 \end{array}$	11054.39	(0.10)	3(1, 2) - 3(0, 3)		A	[70069]
	11055.23	(0.10)	3(1, 2) - 3(0, 3)		E	[70069]
	13471.43	(0.10)	4(1, 3) - 4(0, 4)	1	A	[70069]
	13510.06	(0.10)	4(1, 3) - 4(0, 4)		E	[70069]
	13510.82	(0.10)	4(1, 3) - 4(0, 4)		A	[70069]
	14085.49	(0.10)	2(1, 2) - 1(1, 1)	1	A	[70069]
	14095.49	(0.10)	2(1, 2) - 1(1, 1)		A	[70069]
	14130.43	(0.10)	2(1, 2) - 1(1, 1)	1	E	[70069]
	14929.44	(0.10)	2(0, 2) - 1(0, 1)	1	A	[70069]
	14941.76	(0.10)	2(0, 2) - 1(0, 1)		A	[70069]
	15890.04	(0.10)	2(1, 2) - 1(1, 1)	1	E	[70069]
	15935.08	(0.10)	2(1, 1) - 1(1, 0)	1	A	[70069]
	15950.48	(0.10)	2(1, 1) - 1(1, 0)		A	[70069]
	16841.04	(0.10)	5(1, 4) - 5(0, 5)	1	A	[70069]
	16875.26	(0.10)	5(1, 4) - 5(0, 5)	1	E	[70069]
	16889.58	(0.10)	5(1, 4) - 5(0, 5)		E	[70069]
	16890.25	(0.10)	5(1, 4) - 5(0, 5)		A	[70069]
	19790.89	(0.10)	5(2, 3) - 5(1, 4)	1	A	[70069]
	19810.48	(0.10)	6(2, 4) - 6(1, 5)		E	[70069]
	19812.48	(0.10)	6(2, 4) - 6(1, 5)		A	[70069]
	19845.72	(0.10)	5(2, 3) - 5(1, 4)		E	[70069]
	19848.00	(0.10)	5(2, 3) - 5(1, 4)		A	[70069]
	20421.28	(0.10)	4(2, 2) - 4(1, 3)	1	A	[70069]
	20477.62	(0.10)	4(2, 2) - 4(1, 3)		E	[70069]
	20479.91	(0.10)	4(2, 2) - 4(1, 3)		A	[70069]
	20528.95	(0.10)	7(2, 5) - 7(1, 6)	1	A	[70069]
	20586.45	(0.10)	7(2, 5) - 7(1, 6)		E	[70069]
	20588.71	(0.10)	7(2, 5) - 7(1, 6)		A	[70069]
21079.69	(0.10)	3(1, 3) - 2(1, 2)	1	A	[70069]	
21092.02	(0.10)	3(1, 3) - 2(1, 2)	1	E	[70069]	
21094.46	(0.10)	3(1, 3) - 2(1, 2)		A	[70069]	
21235.21	(0.10)	6(1, 5) - 6(0, 6)		E	[70069]	
21235.96	(0.10)	6(1, 5) - 6(0, 6)		A	[70069]	
21383.32	(0.10)	3(2, 1) - 3(1, 2)	1	E	[70069]	
21442.57	(0.10)	3(2, 1) - 3(1, 2)		E	[70069]	
21444.73	(0.10)	3(2, 1) - 3(1, 2)		A	[70069]	
21524.20	(0.10)	2(1, 2) - 1(0, 1)	1	A	[70069]	
21534.58	(0.10)	2(1, 2) - 1(0, 1)	1	E	[70069]	
21554.89	(0.10)	2(1, 2) - 1(0, 1)		E	[70069]	
21555.74	(0.10)	2(1, 2) - 1(0, 1)		A	[70069]	
22195.52	(0.10)	3(0, 3) - 2(0, 2)	1	A	[70069]	
22196.83	(0.10)	3(0, 3) - 2(0, 2)	1	E	[70069]	
22213.70	(0.10)	3(0, 3) - 2(0, 2)		A	[70069]	
22515.37	(0.10)	3(2, 2) - 2(2, 1)	1	A	[70069]	
22534.38	(0.10)	3(2, 2) - 2(2, 1)		A	[70069]	
22535.89	(0.10)	3(2, 2) - 2(2, 1)		E	[70069]	
22641.57	(0.10)	3(2, 2) - 2(2, 1)	1	E	[70069]	
22707.48	(0.10)	3(2, 1) - 2(2, 0)	1	E	[70069]	
22835.17	(0.10)	3(2, 1) - 2(2, 0)	1	A	[70069]	
22853.51	(0.10)	3(2, 1) - 2(2, 0)		E	[70069]	
22855.15	(0.10)	3(2, 1) - 2(2, 0)		A	[70069]	
23837.44	(0.10)	3(1, 2) - 2(1, 1)	1	E	[70069]	
23848.81	(0.10)	3(1, 2) - 2(1, 1)	1	A	[70069]	
23872.44	(0.10)	3(1, 2) - 2(1, 1)		A	[70069]	
25108.70	(0.10)	9(2, 7) - 9(1, 8)	1	A	[70069]	
25158.84	(0.10)	2(2, 1) - 2(1, 2)		E	[70069]	
25160.98	(0.10)	9(2, 7) - 9(1, 8)	1	E	[70069]	
25163.45	(0.10)	2(2, 1) - 2(1, 2)		A	[70069]	
25180.70	(0.10)	9(2, 7) - 9(1, 8)		E	[70069]	
25181.72	(0.10)	9(2, 7) - 9(1, 8)		A	[70069]	
26462.96	(0.10)	7(1, 6) - 7(0, 7)		E	[70069]	
26463.72	(0.10)	7(1, 6) - 7(0, 7)		A	[70069]	
26526.51	(0.10)	3(2, 2) - 3(1, 3)	1	A	[70069]	
26600.21	(0.10)	3(2, 2) - 3(1, 3)		E	[70069]	
26603.19	(0.10)	3(2, 2) - 3(1, 3)		A	[70069]	

TABLE 45.2. Microwave spectrum of 1-methylcyclobutene — Continued

C₅H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_1	Sym.	Ref.
	27674.61	(0.10)	3(1, 3) - 2(0, 2)	1	A	[70069]
	27697.07	(0.10)	3(1, 3) - 2(0, 2)	1	E	[70069]
	27707.75	(0.10)	3(1, 3) - 2(0, 2)		E	[70069]
	27708.61	(0.10)	3(1, 3) - 2(0, 2)		A	[70069]
	28021.59	(0.10)	4(1, 4) - 3(1, 3)	1	A	[70069]
	28026.89	(0.10)	4(1, 4) - 3(1, 3)	1	E	[70069]
	28040.95	(0.10)	4(1, 4) - 3(1, 3)		A	[70069]
	28541.86	(0.10)	4(2, 3) - 4(1, 4)		E	[70069]
	28544.67	(0.10)	4(2, 3) - 4(1, 4)		A	[70069]
	29079.75	(0.10)	10(2, 8) - 10(1, 9)	1	A	[70069]
	29113.96	(0.10)	10(2, 8) - 10(1, 9)	1	E	[70069]
	29164.33	(0.10)	10(2, 8) - 10(1, 9)		E	[70069]
	29164.91	(0.10)	10(2, 8) - 10(1, 9)		A	[70069]
	29245.66	(0.10)	4(0, 4) - 3(0, 3)	1	A	[70069]
	29248.49	(0.10)	4(0, 4) - 3(0, 3)	1	E	[70069]
	29268.65	(0.10)	4(0, 4) - 3(0, 3)		A	[70069]
	29936.95	(0.10)	11(3, 8) - 11(2, 9)	1	A	[70069]
	29957.32	(0.10)	4(2, 3) - 3(2, 2)	1	A	[70069]
	29982.54	(0.10)	4(2, 3) - 3(2, 2)		A	[70069]
	30018.74	(0.10)	11(3, 8) - 11(2, 9)		E	[70069]
	30021.78	(0.10)	11(3, 8) - 11(2, 9)		A	[70069]
	30120.40	(0.10)	4(2, 3) - 3(2, 2)	1	E	[70069]
	30123.08	(0.10)	10(3, 7) - 10(2, 8)	1	A	[70069]
	30169.72	(0.10)	4(3, 2) - 3(3, 1)	1	A	[70069]
	30180.89	(0.10)	4(3, 1) - 3(3, 0)	1	E	[70069]
	30195.47	(0.10)	4(3, 2) - 3(3, 1)		A	[70069]
	30195.90	(0.10)	4(3, 1) - 3(3, 0)	1	A	[70069]
	30203.53	(0.10)	4(3, 2) - 3(3, 1)		E	[70069]
	30204.28	(0.10)	10(3, 7) - 10(2, 8)		E	[70069]
	30207.92	(0.10)	10(3, 7) - 10(2, 8)		A	[70069]
	30214.26	(0.10)	4(3, 1) - 3(3, 0)		E	[70069]
	30222.08	(0.10)	4(3, 1) - 3(3, 0)		A	[70069]
	30341.91	(0.10)	10(3, 7) - 10(2, 8)	1	E	[70069]
	30569.18	(0.10)	4(2, 2) - 3(2, 1)	1	E	[70069]
	30731.93	(0.10)	4(2, 2) - 3(2, 1)	1	A	[70069]
	30759.44	(0.10)	4(2, 2) - 3(2, 1)		A	[70069]
	30820.89	(0.10)	12(3, 9) - 12(2, 10)	1	A	[70069]
	30906.53	(0.10)	12(3, 9) - 12(2, 10)		E	[70069]
	30908.90	(0.10)	12(3, 9) - 12(2, 10)		A	[70069]
	30942.68	(0.10)	12(3, 9) - 12(2, 10)	1	E	[70069]
	30990.92	(0.10)	5(2, 4) - 5(1, 5)		E	[70069]
	30994.53	(0.10)	5(2, 4) - 5(1, 5)		A	[70069]
	31155.91	(0.10)	9(3, 6) - 9(2, 7)	1	A	[70069]
	31239.54	(0.10)	9(3, 6) - 9(2, 7)		E	[70069]
	31243.58	(0.10)	9(3, 6) - 9(2, 7)		A	[70069]
	31456.75	(0.10)	9(3, 6) - 9(2, 7)	1	E	[70069]
	31689.91	(0.10)	4(1, 3) - 3(1, 2)	1	E	[70069]
	31693.96	(0.10)	4(1, 3) - 3(1, 2)	1	A	[70069]
	31724.41	(0.10)	4(1, 3) - 3(1, 2)		A	[70069]
	31791.25	(0.10)	5(0, 5) - 4(1, 4)	1	E	[70069]
	31810.04	(0.10)	5(0, 5) - 4(1, 4)	1	A	[70069]
	31825.21	(0.10)	5(0, 5) - 4(1, 4)		A	[70069]
	31825.94	(0.10)	5(0, 5) - 4(1, 4)		E	[70069]
	33535.01	(0.10)	4(1, 4) - 3(0, 3)		E	[70069]
	33535.91	(0.10)	4(1, 4) - 3(0, 3)		A	[70069]
	34903.03	(0.10)	5(1, 5) - 4(1, 4)	1	A	[70069]
	34906.41	(0.10)	5(1, 5) - 4(1, 4)	1	E	[70069]
	34926.94	(0.10)	5(1, 5) - 4(1, 4)		A	[70069]
	36064.99	(0.10)	5(0, 5) - 4(0, 4)	1	E	[70069]
	36069.70	(0.10)	5(0, 5) - 4(0, 4)	1	A	[70069]
	36092.22	(0.10)	5(0, 5) - 4(0, 4)		A	[70069]
	37759.54	(0.10)	5(3, 3) - 4(3, 2)	1	A	[70069]
	37792.32	(0.10)	5(3, 3) - 4(3, 2)		A	[70069]
	37798.19	(0.10)	5(3, 3) - 4(3, 2)		E	[70069]
	37851.50	(0.10)	5(3, 2) - 4(3, 1)	1	A	[70069]
	37877.76	(0.10)	5(3, 2) - 4(3, 1)		E	[70069]
	37884.24	(0.10)	5(3, 2) - 4(3, 1)		A	[70069]

Table 46.1. Molecular constants for 1,1-dimethylallene in the ground vibrational state.

Parameter	$(\text{CH}_3)_2\text{C}=\text{C}=\text{CH}_2$ [76060]
\tilde{A} (MHz)	8263.99082(298)
\tilde{B} (MHz)	3614.19398(136)
\tilde{C} (MHz)	2639.48826(89)
Δ_J (MHz)	$0.4970(95)\times 10^{-3}$
Δ_{JK} (MHz)	$0.010490(60)\times 10^{-3}$
Δ_K (MHz)	$1.985(204)\times 10^{-3}$
δ_J (MHz)	$0.15723(173)\times 10^{-3}$
δ_K (MHz)	$6.108(40)\times 10^{-3}$
<u>Internal Rotation Constants [71050]</u>	
I_α (u \AA^2)	3.13 (assumed)
θ	52.8°
s	56.66(6)
V_3 (cm^{-1})	708.7(11)
<u>Dipole Moment [71050]</u>	
μ_a (D)	0.549(1)

Table 46.2. Rotational constants for excited vibrational states of 1,1-dimethylallene. [77040]

State	A (MHz)	B (MHz)	C (MHz)	E (cm^{-1})
ν_I^a	8259.16(20)	3617.640(20)	2640.214(20)	-191.
ν_{II}^a	8248.25(10)	3626.382(20)	2640.565(20)	
ν_{16}	8251.23(20)	3613.797(3)	2638.384(3)	-236.
ν_{32}	8270.73(4)	3618.352(5)	2643.832(5)	-241.
$2\nu_{32}$	8274.1(25)	3622.60(9)	2648.28(1)	--
ν_{11}	8206.9(5)	3621.87(2)	2639.99(1)	-355.

^aCoriolis perturbation analysis yields the constants $D=5989.38(40)$ MHz and $\Delta E_{II,I} = 48761.2(10)$ MHz.

TABLE 46.3. Microwave spectrum of dimethylallene

C₃H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Sym.	Vib. state	Ref.
(CH ₃) ₂ CCCH ₂	6248.88	(0.05)	28(9,19) - 28(9,20)			[76060]
	9976.06	(0.05)	9(3, 6) - 9(3, 7)	EE	1ν _I	[76060]
H ₃ C \ C=C=CH ₂	11523.34	(0.05)	14(4,10) - 14(4,11)	EE	1ν _{II}	[77040]
H ₃ C	11532.64	(0.05)	2(1, 2) - 1(1, 1)			[71050]
	11541.830	(0.050)	2(1, 2) - 1(1, 1)		1ν ₁₁	[71050]
	11549.84	(0.05)	2(1, 2) - 1(1, 1)	EE	1ν ₃₂	[77040]
	11564.87	(0.05)	2(1, 2) - 1(1, 1)	EE	1ν _I	[77040]
	11578.42	(0.05)	2(1, 2) - 1(1, 1)	EE	1ν _{II}	[77040]
	12014.68	(0.05)	12(4, 8) - 12(4, 9)	EE	1ν _I	[77040]
	12361.66	(0.05)	2(0, 2) - 1(0, 1)	EE	1ν _I	[77040]
	12365.69	(0.05)	2(0, 2) - 1(0, 1)	A ₂ A ₁	1ν ₁₆	[77040]
	12366.03	(0.05)	2(0, 2) - 1(0, 1)	EE	1ν ₁₆	[77040]
	12366.44	(0.05)	2(0, 2) - 1(0, 1)	AE + EA	1ν ₁₆	[77040]
	12369.58	(0.05)	2(0, 2) - 1(0, 1)			[71050]
	12382.250	(0.050)	2(0, 2) - 1(0, 1)		1ν ₁₁	[77040]
	12386.68	(0.05)	2(0, 2) - 1(0, 1)	EE	1ν ₃₂	[77040]
	12420.32	(0.05)	2(0, 2) - 1(0, 1)	EE	1ν _{II}	[77040]
	13462.64	(0.05)	2(1, 1) - 1(1, 0)	EE	1ν _I	[77040]
	13478.95	(0.05)	2(1, 1) - 1(1, 0)	A ₂ A ₁	1ν ₁₆	[77040]
	13479.64	(0.05)	2(1, 1) - 1(1, 0)	EE	1ν ₁₆	[77040]
	13480.33	(0.05)	2(1, 1) - 1(1, 0)	AE + EA	1ν ₁₆	[77040]
	13481.98	(0.05)	2(1, 1) - 1(1, 0)			[71050]
	13493.08	(0.05)	2(1, 1) - 1(1, 0)	EE	1ν _{II}	[77040]
	13498.73	(0.05)	2(1, 1) - 1(1, 0)	EE	1ν ₃₂	[77040]
	13505.480	(0.050)	2(1, 1) - 1(1, 0)		1ν ₁₁	[77040]
	13673.57	(0.05)	8(1, 7) - 7(3, 4)			[76060]
	13762.286	(0.080)	23(7,16) - 23(7,17)	AE + EA		[71050]
	13762.837	(0.080)	23(7,16) - 23(7,17)	EE		[71050]
	13763.368	(0.080)	23(7,16) - 23(7,17)	AA		[71050]
	14272.59	(0.05)	15(4,11) - 15(4,12)	EE	1ν _I	[77040]
	15419.158	(0.080)	20(6,14) - 20(6,15)	AE + EA		[71050]
	15419.661	(0.080)	20(6,14) - 20(6,15)	EE		[71050]
	15420.174	(0.080)	20(6,14) - 20(6,15)	AA		[71050]
	16034.36	(0.08)	10(2, 8) - 9(4, 5)			[76060]
	16459.89	(0.05)	8(2, 6) - 8(2, 7)	EE	1ν _{II}	[77040]
	16594.39	(0.05)	8(2, 6) - 8(2, 7)			[71050]
	16722.28	(0.05)	17(5,12) - 17(5,13)	EE	1ν ₃₂	[77040]
	16725.13	(0.05)	17(5,12) - 17(5,13)	EE	1ν ₃₂	[77040]
	16727.95	(0.05)	17(5,12) - 17(5,13)	EE	1ν ₃₂	[77040]
	16750.943	(0.080)	17(5,12) - 17(5,13)	AE + EA		[71050]
	16751.419	(0.080)	17(5,12) - 17(5,13)	EE		[71050]
	16751.890	(0.080)	17(5,12) - 17(5,13)	AA		[71050]
	16863.49	(0.05)	17(5,12) - 17(5,13)	A ₂ A ₁	1ν ₁₆	[77040]
	16873.55	(0.05)	17(5,12) - 17(5,13)	EE	1ν ₁₆	[77040]
	16883.62	(0.05)	17(5,12) - 17(5,13)	AE + EA	1ν ₁₆	[77040]
	17033.113	(0.080)	37(11,26) - 37(11,27)	AE + EA		[71050]
	17033.969	(0.080)	37(11,26) - 37(11,27)	EE		[71050]
	17034.842	(0.080)	37(11,26) - 37(11,27)	AA		[71050]
	17212.02	(0.05)	3(1, 3) - 2(1, 2)	A ₂ A ₁	1ν ₁₆	[77040]
	17212.31	(0.05)	3(1, 3) - 2(1, 2)	EE	1ν ₁₆	[77040]
	17212.62	(0.05)	3(1, 3) - 2(1, 2)	AE + EA	1ν ₁₆	[77040]
	17218.19	(0.05)	3(1, 3) - 2(1, 2)			[71050]
	17229.930	(0.050)	3(1, 3) - 2(1, 2)		1ν ₁₁	[77040]
	17244.00	(0.05)	3(1, 3) - 2(1, 2)	EE	1ν ₃₂	[77040]
	17253.80	(0.05)	3(1, 3) - 2(1, 2)	EE	1ν _I	[77040]
	17269.87	(0.05)	3(1, 3) - 2(1, 2)	AE + EA	2ν ₃₂	[77040]
	17270.26	(0.05)	3(1, 3) - 2(1, 2)	EE	2ν ₃₂	[77040]
	17270.62	(0.05)	3(1, 3) - 2(1, 2)	AA	2ν ₃₂	[77040]
	17311.34	(0.05)	3(1, 3) - 2(1, 2)	EE	1ν ₁₁	[77040]
	17525.60	(0.05)	14(4,10) - 14(4,11)	EE	1ν ₃₂	[77040]
	17528.02	(0.05)	14(4,10) - 14(4,11)	EE	1ν ₃₂	[77040]
	17530.49	(0.05)	14(4,10) - 14(4,11)	EE	1ν ₃₂	[77040]
	17547.544	(0.080)	14(4,10) - 14(4,11)	AE + EA		[71050]
	17547.940	(0.080)	14(4,10) - 14(4,11)	EE		[71050]
	17548.345	(0.080)	14(4,10) - 14(4,11)	AA		[71050]
	17564.23	(0.05)	11(3, 8) - 11(3, 9)	EE	1ν ₃₂	[77040]
	17566.20	(0.05)	11(3, 8) - 11(3, 9)	EE	1ν ₃₂	[77040]

TABLE 46.3. Microwave spectrum of dimethylallene — Continued

C₃H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Sym.	Vib. state	Ref.
	17568.17	(0.05)	11(3, 8) - 11(3, 9)	EE	1ν ₃₂	[77040]
	17579.159	(0.080)	11(3, 8) - 11(3, 9)	AE + EA		[71050]
	17579.494	(0.080)	11(3, 8) - 11(3, 9)	EE		[71050]
	17579.832	(0.080)	11(3, 8) - 11(3, 9)	AA		[71050]
	17698.38	(0.05)	13(4, 9) - 13(4, 10)	EE	1ν ₁	[77040]
	17766.73	(0.05)	8(2, 6) - 8(2, 7)	EE	1ν ₁	[77040]
	18007.680	(0.080)	27(8, 19) - 27(8, 20)	AE + EA		[71050]
	18008.362	(0.080)	27(8, 19) - 27(8, 20)	EE		[71050]
	18009.088	(0.080)	27(8, 19) - 27(8, 20)	AA		[71050]
	18181.84	(0.05)	3(0, 3) - 2(0, 2)	EE	1ν ₁	[77040]
	18220.37	(0.05)	3(0, 3) - 2(0, 2)	A ₂ A ₁	1ν ₁₆	[77040]
	18220.80	(0.05)	3(0, 3) - 2(0, 2)	EE	1ν ₁₆	[77040]
	18221.31	(0.05)	3(0, 3) - 2(0, 2)	AE + EA	1ν ₁₆	[77040]
	18227.25	(0.05)	3(0, 3) - 2(0, 2)			[71050]
	18238.250	(0.050)	3(0, 3) - 2(0, 2)		1ν ₁₁	[77040]
	18353.20	(0.05)	3(0, 3) - 2(0, 2)	EE	1ν ₃₂	[77040]
	18357.82	(0.05)	3(0, 3) - 2(0, 2)	EE	1ν ₁₁	[77040]
	18611.37	(0.05)	6(1, 5) - 6(1, 6)	EE	1ν ₁	[77040]
	18741.60	(0.05)	6(1, 5) - 6(1, 6)	EE	1ν ₁₁	[77040]
	18755.51	(0.05)	3(2, 2) - 2(2, 1)	EE	1ν ₁	[77040]
	18760.73	(0.05)	3(2, 2) - 2(2, 1)			[71050]
	18786.23	(0.05)	3(2, 2) - 2(2, 1)	EE	1ν ₃₂	[77040]
	18807.23	(0.05)	3(2, 2) - 2(2, 1)	EE	1ν ₁₁	[77040]
	19138.75	(0.05)	18(5, 13) - 17(7, 10)			[76060]
	19261.60	(0.05)	3(2, 1) - 2(2, 0)	EE	1ν ₁₁	[77040]
	19294.45	(0.05)	3(2, 1) - 2(2, 0)			[71050]
	19319.30	(0.05)	3(2, 1) - 2(2, 0)	EE	1ν ₃₂	[77040]
	19508.79	(0.08)	6(1, 5) - 6(1, 6)			[71050]
	19817.634	(0.080)	34(10,24) - 34(10,25)	AE + EA		[71050]
	19818.540	(0.080)	34(10,24) - 34(10,25)	EE		[71050]
	19819.472	(0.080)	34(10,24) - 34(10,25)	AA		[71050]
	19918.52	(0.05)	34(10,24) - 34(10,25)			[76060]
	20083.13	(0.05)	3(1, 2) - 2(1, 1)	EE	1ν ₁	[77040]
	20124.99	(0.05)	3(1, 2) - 2(1, 1)	A ₂ A ₁	1ν ₁₆	[77040]
	20126.00	(0.05)	3(1, 2) - 2(1, 1)	EE	1ν ₁₆	[77040]
	20126.98	(0.05)	3(1, 2) - 2(1, 1)	AE + EA	1ν ₁₆	[77040]
	20129.84	(0.05)	3(1, 2) - 2(1, 1)			[71050]
	20155.19	(0.05)	3(1, 2) - 2(1, 1)	EE	1ν ₃₂	[77040]
	20162.720	(0.050)	3(1, 2) - 2(1, 1)		1ν ₁₁	[77040]
	20171.94	(0.05)	3(1, 2) - 2(1, 1)	EE	1ν ₁₁	[77040]
	20218.063	(0.080)	24(7, 17) - 24(7, 18)	AE + EA		[71050]
	20218.775	(0.080)	24(7, 17) - 24(7, 18)	EE		[71050]
	20219.475	(0.080)	24(7, 17) - 24(7, 18)	AA		[71050]
	21450.58	(0.05)	11(3, 8) - 11(3, 9)	EE	1ν ₁	[77040]
	21528.29	(0.05)	5(2, 4) - 5(0, 5)	EE	1ν ₁	[77040]
	22015.75	(0.05)	9(2, 7) - 9(2, 8)	EE	1ν ₁₁	[77040]
	22092.64	(0.05)	13(3, 10) - 12(5, 7)			[76060]
	22107.438	(0.080)	21(6, 15) - 21(6, 16)	AE + EA		[71050]
	22108.089	(0.080)	21(6, 15) - 21(6, 16)	EE		[71050]
	22108.749	(0.080)	21(6, 15) - 21(6, 16)	AA		[71050]
	22236.94	(0.05)	11(2, 9) - 10(4, 6)			[76060]
	22341.71	(0.05)	9(2, 7) - 9(2, 8)	EE	1ν ₃₂	[77040]
	22343.57	(0.05)	9(2, 7) - 9(2, 8)	EE	1ν ₃₂	[77040]
	22345.47	(0.05)	9(2, 7) - 9(2, 8)	EE	1ν ₃₂	[77040]
	22350.32	(0.05)	4(2, 3) - 4(0, 4)			[76060]
	22378.88	(0.05)	9(2, 7) - 9(2, 8)	A ₂ A ₁	1ν ₁₆	[77040]
	22385.35	(0.05)	9(2, 7) - 9(2, 8)	EE	1ν ₁₆	[77040]
	22391.77	(0.05)	9(2, 7) - 9(2, 8)	AE + EA	1ν ₁₆	[77040]
	22814.19	(0.05)	4(1, 4) - 3(1, 3)	A ₂ A ₁	1ν ₁₆	[77040]
	22814.56	(0.05)	4(1, 4) - 3(1, 3)	EE	1ν ₁₆	[77040]
	22814.93	(0.05)	4(1, 4) - 3(1, 3)	AE + EA	1ν ₁₆	[77040]
	22822.82	(0.05)	4(1, 4) - 3(1, 3)			[71050]
	22826.972	(0.080)	31(9, 22) - 31(9, 23)	AE + EA		[71050]
	22827.913	(0.080)	31(9, 22) - 31(9, 23)	EE		[71050]
	22828.833	(0.080)	31(9, 22) - 31(9, 23)	AA		[71050]
	22835.390	(0.050)	4(1, 4) - 3(1, 3)		1ν ₁₁	[77040]
	22852.15	(0.05)	4(1, 4) - 3(1, 3)	EE	1ν ₁	[77040]

TABLE 46.3. Microwave spectrum of dimethylallene — Continued

C₃H₃

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Sym.	Vib. state	Ref.
	22857.41	(0.05)	4(1, 4) - 3(1, 3)	EE	1ν ₃₂	[77040]
	22891.90	(0.05)	4(1, 4) - 3(1, 3)	AE + EA	2ν ₃₂	[77040]
	22892.37	(0.05)	4(1, 4) - 3(1, 3)	EE	2ν ₃₂	[77040]
	22892.80	(0.05)	4(1, 4) - 3(1, 3)	AA	2ν ₃₂	[77040]
	22993.87	(0.05)	4(1, 4) - 3(1, 3)	EE	1ν ₁₁	[77040]
	23438.77	(0.05)	18(5,13) - 18(5,14)	EE	1ν ₃₂	[77040]
	23442.32	(0.05)	18(5,13) - 18(5,14)	EE	1ν ₃₂	[77040]
	23445.78	(0.05)	18(5,13) - 18(5,14)	EE	1ν ₃₂	[77040]
	23473.106	(0.080)	18(5,13) - 18(5,14)	AE + EA		[71050]
	23473.692	(0.080)	18(5,13) - 18(5,14)	EE		[71050]
	23474.294	(0.080)	18(5,13) - 18(5,14)	AA		[71050]
	23606.27	(0.05)	18(5,13) - 18(5,14)	A ₂ A ₁	1ν ₁₆	[77040]
	23618.73	(0.05)	18(5,13) - 18(5,14)	EE	1ν ₁₆	[77040]
	23631.13	(0.05)	18(5,13) - 18(5,14)	AE + EA	1ν ₁₆	[77040]
	23681.59	(0.05)	4(0, 4) - 3(0, 3)	EE	1ν ₁	[77040]
	23765.62	(0.05)	4(0, 4) - 3(0, 3)	A ₂ A ₁	1ν ₁₆	[77040]
	23766.02	(0.05)	4(0, 4) - 3(0, 3)	EE	1ν ₁₆	[77040]
	23766.51	(0.05)	4(0, 4) - 3(0, 3)	AE + EA	1ν ₁₆	[77040]
	23773.80	(0.05)	9(2, 7) - 9(2, 8)	EE	1ν ₁	[77040]
	23775.97	(0.05)	4(0, 4) - 3(0, 3)			[71050]
	23780.190	(0.050)	4(0, 4) - 3(0, 3)		1ν ₁₁	[77040]
	23810.90	(0.05)	4(0, 4) - 3(0, 3)	EE	1ν ₃₂	[77040]
	23845.89	(0.05)	4(0, 4) - 3(0, 3)	AE + EA	2ν ₃₂	[77040]
	23846.45	(0.05)	4(0, 4) - 3(0, 3)	EE	2ν ₃₂	[77040]
	23846.96	(0.05)	4(0, 4) - 3(0, 3)	AA	2ν ₃₂	[77040]
	24024.82	(0.05)	4(0, 4) - 3(0, 3)	EE	1ν ₁₁	[77040]
	24055.82	(0.05)	6(2, 5) - 6(0, 6)	EE	1ν ₁	[77040]
	24230.90	(0.05)	5(2, 4) - 5(0, 5)			[76060]
	24560.85	(0.05)	14(4,10) - 14(4,11)	EE	1ν ₁	[77040]
	24712.33	(0.05)	4(2, 3) - 3(2, 2)	EE	1ν ₁₁	[77040]
	24863.45	(0.05)	4(2, 3) - 3(2, 2)	EE	1ν ₁	[77040]
	24906.63	(0.05)	4(2, 3) - 3(2, 2)			[71050]
	24940.79	(0.05)	4(2, 3) - 3(2, 2)	EE	1ν ₃₂	[77040]
	25256.34	(0.05)	4(3, 2) - 3(3, 1)			[71050]
	25265.69	(0.05)	4(3, 2) - 3(3, 1)	EE	1ν ₁	[77040]
	25285.42	(0.05)	4(3, 2) - 3(3, 1)	EE	1ν ₁₁	[77040]
	25329.05	(0.05)	4(3, 1) - 3(3, 0)			[71050]
	25337.76	(0.05)	4(3, 1) - 3(3, 0)	EE	1ν ₁₁	[77040]
	25352.76	(0.05)	4(3, 1) - 3(3, 0)	EE	1ν ₁	[77040]
	25593.515	(0.080)	28(8,20) - 28(8,21)	AE + EA		[71050]
	25594.427	(0.080)	28(8,20) - 28(8,21)	EE		[71050]
	25595.341	(0.080)	28(8,20) - 28(8,21)	AA		[71050]
	25616.95	(0.05)	4(4, 0) - 3(2, 2)		1ν ₁ → 1ν ₁₁	[77040]
	25945.92	(0.05)	5(2, 4) - 5(0, 5)	EE	1ν ₁₁	[77040]
	26144.32	(0.05)	4(2, 2) - 3(2, 1)			[71050]
	26188.04	(0.05)	4(2, 2) - 3(2, 1)	EE	1ν ₁₁	[77040]
	26239.78	(0.05)	4(2, 2) - 3(2, 1)	EE	1ν ₁	[77040]
	26376.39	(0.05)	12(2,10) - 11(4, 7)			[76060]
	26546.10	(0.05)	4(1, 3) - 3(1, 2)	EE	1ν ₁	[77040]
	26648.54	(0.05)	4(1, 3) - 3(1, 2)			[71050]
	26755.54	(0.05)	4(1, 3) - 3(1, 2)	EE	1ν ₁₁	[77040]
	26863.98	(0.05)	6(2, 5) - 6(0, 6)			[76060]
	27041.33	(0.05)	7(2, 6) - 7(0, 7)	EE	1ν ₁	[77040]
	28027.065	(0.080)	25(7,18) - 25(7,19)	AE + EA		[71050]
	28027.929	(0.080)	25(7,18) - 25(7,19)	EE		[71050]
	28028.793	(0.080)	25(7,18) - 25(7,19)	AA		[71050]
	28167.86	(0.05)	6(2, 5) - 6(0, 6)	EE	1ν ₁₁	[77040]
	28229.78	(0.05)	35(10,25) - 35(10,26)			[76060]
	28331.52	(0.05)	5(1, 5) - 4(1, 4)	A ₂ A ₁	1ν ₁₆	[77040]
	28331.91	(0.05)	5(1, 5) - 4(1, 4)	EE	1ν ₁₆	[77040]
	28332.33	(0.05)	5(1, 5) - 4(1, 4)	AE + EA	1ν ₁₆	[77040]
	28342.76	(0.05)	5(1, 5) - 4(1, 4)			[71050]
	28354.651	(0.050)	5(1, 5) - 4(1, 4)		1ν ₁₁	[77040]
	28359.40	(0.05)	5(1, 5) - 4(1, 4)	EE	1ν ₁	[77040]
	28386.11	(0.05)	5(1, 5) - 4(1, 4)	EE	1ν ₃₂	[77040]
	28429.35	(0.05)	5(1, 5) - 4(1, 4)	AE + EA	2ν ₃₂	[77040]
	28429.84	(0.05)	5(1, 5) - 4(1, 4)	EE	2ν ₃₂	[77040]

TABLE 46.3. Microwave spectrum of dimethylallene — Continued

C₃H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Sym.	Vib. state	Ref.
	28430.26	(0.05)	5(1, 5) - 4(1, 4)	AA	2ν ₃₂	[77040]
	28482.63	(0.05)	12(3, 9) - 12(3, 10)	EE	1ν ₁	[77040]
	28501.71	(0.05)	10(2, 8) - 10(2, 9)	EE	1ν ₃₂	[77040]
	28503.87	(0.05)	10(2, 8) - 10(2, 9)	EE	1ν ₃₂	[77040]
	28506.08	(0.05)	10(2, 8) - 10(2, 9)	EE	1ν ₃₂	[77040]
	28537.15	(0.05)	10(2, 8) - 10(2, 9)	A ₂ A ₁	1ν ₁₆	[77040]
	28544.75	(0.05)	10(2, 8) - 10(2, 9)	EE	1ν ₁₆	[77040]
	28552.41	(0.05)	10(2, 8) - 10(2, 9)	AE + EA	1ν ₁₆	[77040]
	28653.78	(0.05)	5(1, 5) - 4(1, 4)	EE	1ν ₁₁	[77040]
	28958.60	(0.05)	5(0, 5) - 4(0, 4)	EE	1ν ₁	[77040]
	29067.95	(0.05)	5(0, 5) - 4(0, 4)	A ₂ A ₁	1ν ₁₆	[77040]
	29068.33	(0.05)	5(0, 5) - 4(0, 4)	EE	1ν ₁₆	[77040]
	29068.75	(0.05)	5(0, 5) - 4(0, 4)	AE + EA	1ν ₁₆	[77040]
	29125.49	(0.05)	5(0, 5) - 4(0, 4)	EE	1ν ₃₂	[77040]
	29458.53	(0.05)	5(0, 5) - 4(0, 4)	EE	1ν ₁₁	[77040]
	29081.64	(0.05)	5(0, 5) - 4(0, 4)			[71050]
	30037.62	(0.05)	14(3, 11) - 13(5, 8)			[76060]
	30037.65	(0.05)	6(3, 4) - 6(1, 5)	EE	1ν ₁	[77040]
	30561.845	(0.080)	13(3, 10) - 13(3, 11)	AE + EA		[71050]
	30562.307	(0.080)	13(3, 10) - 13(3, 11)	EE		[71050]
	30562.775	(0.080)	13(3, 10) - 13(3, 11)	AA		[71050]
	30848.98	(0.05)	5(2, 4) - 4(2, 3)	EE	1ν ₁	[77040]
	30952.59	(0.05)	5(2, 4) - 4(2, 3)	A ₂ A ₁	1ν ₁₆	[77040]
	30953.61	(0.05)	5(2, 4) - 4(2, 3)	EE	1ν ₁₆	[77040]
	30954.71	(0.05)	5(2, 4) - 4(2, 3)	AE + EA	1ν ₁₆	[77040]
	30962.27	(0.05)	5(2, 4) - 4(2, 3)			[71050]
	31005.23	(0.05)	5(2, 4) - 4(2, 3)	EE	1ν ₃₂	[77040]
	31047.75	(0.05)	5(2, 4) - 4(2, 3)	AE + EA	2ν ₃₂	[77040]
	31049.15	(0.05)	5(2, 4) - 4(2, 3)	EE	2ν ₃₂	[77040]
	31050.53	(0.05)	5(2, 4) - 4(2, 3)	AA	2ν ₃₂	[77040]
	31085.52	(0.05)	8(3, 6) - 8(1, 7)	EE	1ν ₁	[77040]
	31099.38	(0.05)	7(2, 6) - 7(0, 7)	EE	1ν ₁₁	[77040]
	31251.61	(0.05)	19(5, 14) - 19(5, 15)	A ₂ A ₁	1ν ₁₆	[77040]
	31266.21	(0.05)	19(5, 14) - 19(5, 15)	EE	1ν ₁₆	[77040]
	31280.72	(0.05)	19(5, 14) - 19(5, 15)	AE + EA	1ν ₁₆	[77040]
	31344.66	(0.05)	16(4, 12) - 16(4, 13)	EE	1ν ₃₂	[77040]
	31348.16	(0.05)	16(4, 12) - 16(4, 13)	EE	1ν ₃₂	[77040]
	31351.68	(0.05)	16(4, 12) - 16(4, 13)	EE	1ν ₃₂	[77040]
	31372.518	(0.080)	16(4, 12) - 16(4, 13)	AE + EA		[71050]
	31373.107	(0.080)	16(4, 12) - 16(4, 13)	EE		[71050]
	31373.683	(0.080)	16(4, 12) - 16(4, 13)	AA		[71050]
	31564.29	(0.08)	5(4, 2) - 4(4, 0)	AE		[71050]
	31572.06	(0.08)	5(4, 2) - 4(4, 1)	AA + EA		[71050]
	31573.07	(0.08)	5(4, 2) - 4(4, 1)	EE		[71050]
	31573.73	(0.08)	5(4, 2) - 4(4, 1)	AE		[71050]
	31577.30	(0.08)	5(4, 1) - 4(4, 0)	AE		[71050]
	31578.13	(0.08)	5(4, 1) - 4(4, 0)	EE		[71050]
	31579.25	(0.08)	5(4, 1) - 4(4, 0)	AA + EA		[71050]
	31581.89	(0.08)	5(4, 1) - 4(4, 1)	EE		[71050]
	31586.66	(0.08)	5(4, 1) - 4(4, 1)	AE		[71050]
	31609.84	(0.05)	5(3, 3) - 4(3, 2)	EE	1ν ₁	[77040]
	31625.75	(0.05)	5(3, 3) - 4(3, 2)			[71050]
	31650.13	(0.05)	5(3, 3) - 4(3, 2)	EE	1ν ₁₁	[77040]
	31831.41	(0.05)	5(3, 2) - 4(3, 1)	EE	1ν ₁₁	[77040]
	31835.50	(0.05)	5(2, 4) - 4(2, 3)	EE	1ν ₁₁	[77040]
	31873.57	(0.05)	5(3, 2) - 4(3, 1)			[71050]
	31875.89	(0.05)	5(3, 2) - 4(3, 1)	EE	1ν ₁	[77040]
	31915.04	(0.05)	5(3, 2) - 4(3, 1)	EE	1ν ₃₂	[77040]
	32267.43	(0.05)	15(3, 12) - 15(3, 13)	EE	1ν ₁	[77040]
	32391.44	(0.05)	6(3, 3) - 5(1, 5)		1ν ₁ → 1ν ₁₁	[77040]
	32761.27	(0.05)	5(1, 4) - 4(1, 3)	EE	1ν ₁	[77040]
	32957.68	(0.05)	5(1, 4) - 4(1, 3)	A ₂ A ₁	1ν ₁₆	[77040]
	32959.12	(0.05)	5(1, 4) - 4(1, 3)	EE	1ν ₁₆	[77040]
	32960.57	(0.05)	5(1, 4) - 4(1, 3)	AE + EA	1ν ₁₆	[77040]
	32968.06	(0.05)	5(1, 4) - 4(1, 3)			[71050]
	33052.89	(0.05)	5(1, 4) - 4(1, 3)	AE + EA	2ν ₃₂	[77040]
	33053.41	(0.05)	5(1, 4) - 4(1, 3)	EE	2ν ₃₂	[77040]

TABLE 46.3. Microwave spectrum of dimethylallene — Continued

C₃H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Sym.	Vib. state	Ref.
	33053.89	(0.05)	5(1, 4) - 4(1, 3)	AA	2ν ₃₂	[77040]
	33141.51	(0.05)	5(2, 3) - 4(2, 2)			[71050]
	33146.15	(0.05)	5(2, 3) - 4(2, 2)	EE	1ν _{II}	[77040]
	33190.41	(0.05)	5(0, 5) - 4(0, 4)	EE	1ν _{II}	[77040]
	33226.61	(0.05)	5(2, 3) - 4(2, 2)	EE	1ν _I	[77040]
	33786.30	(0.05)	6(1, 6) - 5(1, 5)			[71050]
	33788.47	(0.05)	6(1, 6) - 5(1, 5)	EE	1ν _I	[77040]
	33838.49	(0.05)	6(1, 6) - 5(1, 5)	EE	1ν ₃₂	[77040]
	33890.46	(0.05)	6(1, 6) - 5(1, 5)	AE + EA	2ν ₃₂	[77040]
	33890.98	(0.05)	6(1, 6) - 5(1, 5)	EE	2ν ₃₂	[77040]
	33891.37	(0.05)	6(1, 6) - 5(1, 5)	AA	2ν ₃₂	[77040]
	34021.29	(0.05)	11(2, 9) - 11(2, 10)	EE	1ν _{II}	[77040]
	34157.82	(0.05)	6(0, 6) - 5(0, 5)	EE	1ν _I	[77040]
	34174.91	(0.05)	22(6, 16) - 21(8, 13)			[76060]
	34178.17	(0.05)	7(3, 5) - 7(1, 6)			[76060]
	34260.62	(0.05)	6(0, 6) - 5(0, 5)	A ₂ A ₁	1ν ₁₆	[77040]
	34260.97	(0.05)	6(0, 6) - 5(0, 5)	EE	1ν ₁₆	[77040]
	34261.32	(0.05)	6(0, 6) - 5(0, 5)	AE + EA	1ν ₁₆	[77040]
	34329.62	(0.05)	6(0, 6) - 5(0, 5)	EE	1ν ₃₂	[77040]
	34382.36	(0.05)	6(0, 6) - 5(0, 5)	EE	2ν ₃₂	[77040]
	34382.92	(0.05)	6(0, 6) - 5(0, 5)	AA	2ν ₃₂	[77040]
	34628.94	(0.05)	8(3, 6) - 8(1, 7)			[76060]
	34702.39	(0.05)	6(1, 6) - 5(1, 5)	EE	1ν _{II}	[77040]
	34773.51	(0.05)	6(0, 6) - 5(0, 5)	EE	1ν _{II}	[77040]
	35885.36	(0.05)	13(3, 10) - 13(3, 11)	EE	1ν _I	[77040]
	35993.94	(0.05)	15(3, 12) - 14(5, 9)			[76060]
	36050.05	(0.05)	9(3, 7) - 9(1, 8)			[76060]
	36685.38	(0.05)	6(2, 5) - 5(2, 4)	EE	1ν _I	[77040]
	36909.99	(0.05)	6(2, 5) - 5(2, 4)			[71050]
	36995.53	(0.05)	6(2, 5) - 5(2, 4)	EE	1ν _{II}	[77040]
	37505.55	(0.05)	8(3, 6) - 8(1, 7)	EE	1ν _{II}	[77040]

Table 47.1. Molecular constants for trans- and cis-1,3-pentadiene.

Parameter	trans-CH ₃ CHCHCHCH ₂	cis-CH ₃ CHCHCHCH ₂
A (MHz)	27367.(872)	15662.(62)
B (MHz)	2160.616(4)	2658.391(17)
C (MHz)	2033.212(5)	2306.129(16)
Δ_J (kHz)	0.16(11)	0.51(26)
Δ_{JK} (kHz)	---	-2.5(50)
<u>Internal Rotation Constants</u>		
I_α (u Å ²)	3.13 ^a	3.13 ^a
λ_a	0.9048	0.46947 ^a
θ	25.2 ^a	62.0 ^a
V_3 (cm ⁻¹)	624.0(21)	258.2(5)
s	44.19	20.55
F (GHz)	187.94	167.18
<u>Electric Dipole Moment [70070]</u>		
μ_a (D)	0.561(2)	0.465(10)
μ_b (D)	0.16(3)	0.185(15)

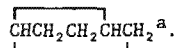
^aAssumed.

TABLE 47.2. Microwave spectrum of 1,3-pentadiene

C₅H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Sym.	Ref.	
<i>t</i> -CH ₃ CHCHCH ₂	8260.24	(0.07)	2(1, 2) - 1(1, 1)	<i>A</i>	[70070]	
	8261.270	(0.070)	2(1, 2) - 1(1, 1)	<i>E</i>	[70070]	
	8387.16	(0.07)	2(0, 2) - 1(0, 1)	<i>A</i>	[70070]	
	8514.003	(0.070)	2(1, 1) - 1(1, 0)	<i>E</i>	[70070]	
	8515.04	(0.07)	2(1, 1) - 1(1, 0)	<i>A</i>	[70070]	
	12390.07	(0.07)	3(1, 3) - 2(1, 2)	<i>A</i>	[70070]	
	12390.327	(0.070)	3(1, 3) - 2(1, 2)	<i>E</i>	[70070]	
	12579.55	(0.07)	3(0, 3) - 2(0, 2)	<i>A</i>	[70070]	
	12581.47	(0.07)	3(2, 2) - 2(2, 1)	<i>A</i>	[70070]	
	12583.40	(0.07)	3(2, 1) - 2(2, 0)	<i>A</i>	[70070]	
	12772.27	(0.07)	3(1, 2) - 2(1, 1)	<i>A</i>	[70070]	
	12772.004	(0.070)	3(1, 2) - 2(1, 1)	<i>E</i>	[70070]	
	16519.60	(0.07)	4(1, 4) - 3(1, 3)	<i>A</i>	[70070]	
	17029.025	(0.070)	4(1, 3) - 3(1, 2)	<i>E</i>	[70070]	
	17029.16	(0.07)	4(1, 3) - 3(1, 2)	<i>A</i>	[70070]	
	20648.41	(0.07)	5(1, 5) - 4(1, 4)	<i>A</i>	[70070]	
	21285.375	(0.070)	5(1, 4) - 4(1, 3)	<i>E</i>	[70070]	
	21285.45	(0.07)	5(1, 4) - 4(1, 3)	<i>A</i>	[70070]	
	24776.80	(0.07)	6(1, 6) - 5(1, 5)	<i>A</i>	[70070]	
	25541.129	(0.070)	6(1, 5) - 5(1, 4)	<i>E</i>	[70070]	
	25541.20	(0.07)	6(1, 5) - 5(1, 4)	<i>A</i>	[70070]	
	<i>c</i> -CH ₃ CHCHCH ₂	9577.53	(0.07)	2(1, 2) - 1(1, 1)	<i>A</i>	[70070]
		9921.04	(0.07)	2(0, 2) - 1(0, 1)	<i>E</i>	[70070]
		9923.50	(0.07)	2(0, 2) - 1(0, 1)	<i>A</i>	[70070]
10283.63		(0.07)	2(1, 1) - 1(1, 0)	<i>A</i>	[70070]	
14361.95		(0.07)	3(1, 3) - 2(1, 2)	<i>A</i>	[70070]	
14369.56		(0.07)	3(1, 3) - 2(1, 2)	<i>E</i>	[70070]	
14863.93		(0.07)	3(0, 3) - 2(0, 2)	<i>E</i>	[70070]	
14867.49		(0.07)	3(0, 3) - 2(0, 2)	<i>A</i>	[70070]	
14895.96		(0.07)	3(2, 2) - 2(2, 1)	<i>A</i>	[70070]	
14924.15		(0.07)	3(2, 1) - 2(2, 0)	<i>A</i>	[70070]	
15406.65		(0.07)	3(1, 2) - 2(1, 1)	<i>E</i>	[70070]	
15420.91		(0.07)	3(1, 2) - 2(1, 1)	<i>A</i>	[70070]	
19141.05		(0.07)	4(1, 4) - 3(1, 3)	<i>A</i>	[70070]	
19142.548		(0.070)	4(1, 4) - 3(1, 3)	<i>E</i>	[70070]	
19785.893		(0.070)	4(0, 4) - 3(0, 3)	<i>E</i>	[70070]	
19790.40		(0.07)	4(0, 4) - 3(0, 3)	<i>A</i>	[70070]	
19855.57		(0.07)	4(2, 3) - 3(2, 2)	<i>A</i>	[70070]	
19926.07		(0.07)	4(2, 2) - 3(2, 1)	<i>A</i>	[70070]	
20542.42		(0.07)	4(1, 3) - 3(1, 2)	<i>E</i>	[70070]	
20552.60		(0.07)	4(1, 3) - 3(1, 2)	<i>A</i>	[70070]	
23912.612		(0.070)	5(1, 5) - 4(1, 4)	<i>E</i>	[70070]	
23913.59		(0.07)	5(1, 5) - 4(1, 4)	<i>A</i>	[70070]	
25666.95		(0.07)	5(1, 4) - 4(1, 3)	<i>E</i>	[70070]	
25676.79		(0.07)	5(1, 4) - 4(1, 3)	<i>A</i>	[70070]	
34701.41	(0.07)	7(2, 6) - 6(2, 5)	<i>A</i>	[70070]		
35893.24	(0.07)	7(1, 6) - 6(1, 5)	<i>A</i>	[70070]		

Table 48.1. Molecular constants for bicyclo[2.1.0]pentane,



Isotopic Species	A (MHz)	B (MHz)	C (MHz)	Reference
Normal	9100.702(4)	6114.090(4)	4781.690(4)	[72064]
1- ¹³ C	8978.86(1)	6089.75(2)	4748.41(2)	[72064]
2- ¹³ C	9003.32(2)	6035.70(2)	4708.81(1)	[72064]
5- ¹³ C	9061.72(2)	5974.72(3)	4706.60(1)	[72064]
1-d ₁	8583.42(1)	5975.33(2)	4657.34(6)	[76052]
2-endo-d ₁	8673.28(1)	5934.14(4)	4650.18(4)	[76052]
2,3-exo-d ₂	8581.75(1)	5661.04(3)	4409.20(2)	[76052]
2,3-endo-d ₂	8268.93(1)	5769.08(2)	4529.48(1)	[76052]
5-exo-d ₁	9093.40(2)	5730.10(2)	4545.03(3)	[76052]
5-endo-d ₁	8725.62(1)	5856.68(2)	4726.13(2)	[76052]
<u>Electric Dipole Moment</u> [72064]				
μ _a (D)	0.00(1)			
μ _c (D)	0.26(1)			

^aCarbon atom 5 is bonded to atoms 1 and 4 of the 4-membered ring. Atom 1 and 4 and 2 and 3 are equivalent.

TABLE 48.2. microwave spectrum of bicyclo[2.1.0]pentane

C₅H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J''(K_{-1}, K_{+1}) - J'(K_{-1}, K_{+1})$	Ref.
CHCH ₂ CH ₂ CHCH ₂	8959.84	(0.05)	2(2, 1) - 2(1, 1)	[72064]
	13312.87	(0.05)	2(2, 0) - 2(1, 2)	[72064]
$\begin{array}{c} \text{H}_2\text{C}-\text{CH}_2 \\ \quad \\ \text{HC}-\text{CH} \\ \backslash \quad / \\ \text{CH}_2 \end{array}$	15214.80	(0.05)	1(1, 0) - 0(0, 0)	[72064]
	17116.71	(0.05)	2(0, 2) - 1(1, 0)	[72064]
	22326.38	(0.05)	5(2, 4) - 5(3, 2)	[72064]
	26952.02	(0.05)	6(2, 5) - 6(3, 3)	[72064]
	27442.97	(0.05)	2(1, 1) - 1(0, 1)	[72064]
¹³ CHCH ₂ CH ₂ CHCH ₂	32439.60	(0.05)	2(2, 0) - 1(1, 0)	[72064]
	33416.22	(0.05)	2(2, 1) - 1(1, 1)	[72064]
	14495.66	(0.10)	4(3, 2) - 4(2, 2)	[72064]
	15068.68	(0.10)	1(1, 0) - 0(0, 0)	[72064]
	16603.59	(0.10)	3(1, 3) - 3(2, 1)	[72064]
	27248.05	(0.10)	2(1, 1) - 1(0, 1)	[72064]
	33026.38	(0.10)	2(2, 1) - 1(1, 1)	[72064]
	22038.08	(0.10)	5(2, 4) - 5(3, 2)	[72064]
	26830.90	(0.10)	6(2, 5) - 6(3, 3)	[72064]
	32054.45	(0.10)	2(2, 0) - 1(1, 0)	[72064]
CH ¹³ CH ₂ CH ₂ CHCH ₂	15039.08	(0.10)	1(1, 0) - 0(0, 0)	[72064]
	16707.03	(0.10)	3(1, 3) - 3(2, 1)	[72064]
	16839.52	(0.10)	2(0, 2) - 1(1, 0)	[72064]
	22209.01	(0.10)	5(2, 4) - 5(3, 2)	[72064]
	26823.10	(0.10)	6(2, 5) - 6(3, 3)	[72064]
	27110.48	(0.10)	2(1, 1) - 1(0, 1)	[72064]
CHCH ₂ CH ₂ CH ¹³ CH ₂	33045.56	(0.10)	2(2, 1) - 1(1, 1)	[72064]
	13271.68	(0.10)	5(3, 3) - 5(2, 3)	[72064]
	15036.55	(0.10)	1(1, 0) - 0(0, 0)	[72064]
	24946.20	(0.10)	3(0, 3) - 2(1, 1)	[72064]
	26985.85	(0.10)	2(1, 1) - 1(0, 1)	[72064]
	32209.14	(0.10)	2(2, 0) - 1(1, 0)	[72064]
CDCH ₂ CH ₂ CHCH ₂	33159.87	(0.10)	2(2, 1) - 1(1, 1)	[72064]
	26707.20	(0.02)	7(5, 3) - 7(4, 3)	[76052]
	27931.54	(0.02)	6(5, 2) - 6(4, 2)	[76052]
	28514.89	(0.02)	5(5, 1) - 5(4, 1)	[76052]
	28620.17	(0.02)	5(5, 0) - 5(4, 2)	[76052]
	30794.85	(0.02)	2(2, 0) - 1(1, 0)	[76052]
	31725.59	(0.02)	2(2, 1) - 1(1, 1)	[76052]
	34983.43	(0.02)	6(6, 1) - 6(5, 1)	[76052]
	36249.93	(0.02)	4(1, 3) - 3(2, 1)	[76052]
	39216.53	(0.02)	3(1, 2) - 2(0, 2)	[76052]
<i>en</i> -CHCHDCH ₂ CHCH ₂	28034.86	(0.02)	7(5, 3) - 7(4, 3)	[76052]
	29107.82	(0.02)	6(5, 2) - 6(4, 2)	[76052]
	29621.40	(0.02)	5(5, 1) - 5(4, 1)	[76052]
	29707.24	(0.02)	5(5, 0) - 5(4, 2)	[76052]
	31026.30	(0.02)	2(2, 0) - 1(1, 0)	[76052]
	31953.96	(0.02)	2(2, 1) - 1(1, 1)	[76052]
	35792.19	(0.02)	4(1, 3) - 3(2, 1)	[76052]
	36319.38	(0.02)	6(6, 1) - 6(5, 1)	[76052]
	39078.74	(0.02)	3(1, 2) - 2(0, 2)	[76052]
	29207.29	(0.02)	7(5, 3) - 7(4, 3)	[76052]
<i>en</i> -CHCH ₂ CH ₂ CHCHD	29941.50	(0.02)	6(5, 2) - 6(4, 2)	[76052]
	30300.78	(0.02)	5(5, 1) - 5(4, 1)	[76052]
	30350.17	(0.02)	5(5, 0) - 5(4, 2)	[76052]
	31176.68	(0.02)	2(2, 0) - 1(1, 0)	[76052]
	32033.54	(0.02)	2(2, 1) - 1(1, 1)	[76052]
	35517.77	(0.02)	4(1, 3) - 3(2, 1)	[76052]
	37113.68	(0.02)	6(6, 1) - 6(5, 1)	[76052]
	38650.54	(0.02)	3(1, 2) - 2(0, 2)	[76052]
	32087.15	(0.02)	2(2, 0) - 1(1, 0)	[76052]
	33010.29	(0.02)	2(2, 1) - 1(1, 1)	[76052]
<i>ex</i> -CHCH ₂ CH ₂ CHCHD	33090.46	(0.02)	4(1, 3) - 3(2, 1)	[76052]
	34049.57	(0.02)	7(5, 3) - 7(4, 3)	[76052]
	34702.28	(0.02)	6(5, 2) - 6(4, 2)	[76052]
	35028.07	(0.02)	5(5, 1) - 5(4, 1)	[76052]
	35067.16	(0.02)	5(5, 0) - 5(4, 2)	[76052]
	38412.11	(0.02)	3(1, 2) - 2(0, 2)	[76052]

TABLE 48.2. microwave spectrum of bicyclo[2.1.0]pentane — Continued

C₅H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
$\begin{array}{c} \text{en-CHCHDCHDCHCH}_2 \\ \square \end{array}$	27255.29	(0.02)	5(5, 1) - 5(4, 1)	[76052]
	27349.97	(0.02)	5(5, 0) - 5(4, 2)	[76052]
	29695.35	(0.02)	2(2, 0) - 1(1, 0)	[76052]
	30575.87	(0.02)	2(2, 1) - 1(1, 1)	[76052]
	33432.82	(0.02)	6(6, 1) - 6(5, 1)	[76052]
	35187.94	(0.02)	4(1, 3) - 3(2, 1)	[76052]
$\begin{array}{c} \text{ex-CHCHDCHDCHCH}_2 \\ \square \end{array}$	37825.28	(0.02)	3(1, 2) - 2(0, 2)	[76052]
	29829.60	(0.02)	7(5, 3) - 7(4, 3)	[76052]
	30478.44	(0.02)	2(2, 0) - 1(1, 0)	[76052]
	30748.95	(0.02)	6(5, 2) - 6(4, 2)	[76052]
	31193.37	(0.02)	5(5, 1) - 5(4, 1)	[76052]
	31260.67	(0.02)	5(5, 0) - 5(4, 2)	[76052]
	31406.29	(0.02)	2(2, 1) - 1(1, 1)	[76052]
	33336.78	(0.02)	4(1, 3) - 3(2, 1)	[76052]
	37600.40	(0.02)	3(1, 2) - 2(0, 2)	[76052]
	38224.17	(0.02)	6(6, 1) - 6(5, 1)	[76052]

Table 49.1. Molecular constants of 3,3-dimethylcyclopropene.

Parameter	Value	Reference
A (MHz)	6872.964(73)	[present]
B (MHz)	5353.250(11)	[present]
C (MHz)	3846.522(11)	[present]
μ_a (D)	0.287(3)	[78029]

TABLE 49.2. Microwave spectrum of 3,3-dimethylcyclopropene

C₅H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
$\begin{array}{c} \text{CHCHC(CH}_3\text{)}_2 \\ \square \end{array}$	27599.39	(0.10)	3(2, 2) - 2(2, 1)	[78029]
	29262.56	(0.10)	3(1, 2) - 2(1, 1)	[78029]
	29754.80	(0.10)	3(2, 1) - 2(2, 0)	[78029]
$\begin{array}{c} \text{HC=CH} \\ \backslash / \\ \text{C} \\ / \backslash \end{array}$	32832.34	(0.10)	4(1, 4) - 3(1, 3)	[78029]
	33003.42	(0.10)	4(0, 4) - 3(0, 3)	[78029]
	36228.39	(0.10)	4(2, 3) - 3(2, 2)	[78029]
	37727.62	(0.10)	4(1, 3) - 3(1, 2)	[78029]
$\begin{array}{c} \text{H}_3\text{C} \quad \text{CH}_3 \\ \square \end{array}$	37752.38	(0.10)	4(3, 2) - 3(3, 1)	[78029]
	38883.89	(0.10)	4(3, 1) - 3(3, 0)	[78029]

Table 50.1. Molecular constants for cyclopentene in the ground state and excited out-of-plane bending state. [65035]

Vibrational State	v	A (MHz)	B (MHz)	C (MHz)	μ_b (D)
<u>CH₂(CH₂)₃CH₂</u>					
Ground ^a		7298.53	7227.57	3948.78	0.190(6)
	1 ^a	7289.03	7228.50	3950.46	0.193(11)
	2	7281.28	7202.98	3915.78	
	3	7285.80	7218.36	3939.73	

^aThese were fit together with the vibration rotation parameters $\delta_{01} = 1.34 \times 10^5 \text{ MHz}^2/\text{s}^2$ and $E_1 - E_0 = 27300 \text{ MHz}$.

TABLE 50.2. Microwave spectrum of cyclopentene

C₅H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
CHCHCH ₂ CH ₂ CH ₂	8209.99	(0.10)	14(13, 1) - 14(12, 2)	1ν ₁	[62023]
	8218.95	(0.10)	15(14, 1) - 15(13, 2)	1ν ₁	[62023]
$ \begin{array}{c} \text{HC}=\text{CH} \\ \quad \\ \text{H}_2\text{C} \quad \text{CH}_2 \\ \quad \quad \backslash \\ \quad \quad \text{CH}_2 \end{array} $	8249.79	(0.10)	13(12, 1) - 13(11, 2)	1ν ₁	[62023]
	8281.85	(0.10)	16(15, 1) - 16(14, 2)	1ν ₁	[62023]
	8309.34	(0.10)	14(13, 1) - 14(12, 2)	3ν ₁	[62023]
	8320.2	(0.3)	14(13, 1) - 14(12, 2)	4ν ₁	[62023]
	8327.5	(0.3)	13(12, 1) - 13(11, 2)	3ν ₁	[62023]
	8327.5	(0.3)	13(12, 1) - 13(11, 2)	4ν ₁	[62023]
	8332.21	(0.10)	12(11, 1) - 12(10, 2)	1ν ₁	[62023]
	8344.1	(0.3)	15(14, 1) - 15(13, 2)	3ν ₁	[62023]
	8345.22	(0.3)	13(12, 1) - 13(11, 2)	2ν ₁	[62023]
	8365.88	(0.10)	12(11, 1) - 12(10, 2)	2ν ₁	[62023]
	8368.4	(0.3)	15(14, 1) - 15(13, 2)	4ν ₁	[62023]
	8385.1	(0.3)	12(11, 1) - 12(10, 2)	4ν ₁	[62023]
	8386.41	(0.3)	14(13, 1) - 14(12, 2)	2ν ₁	[62023]
	8392.3	(0.3)	12(11, 1) - 12(10, 2)	3ν ₁	[62023]
	8402.47	(0.3)	17(16, 1) - 17(15, 2)	1ν ₁	[62023]
	8437.9	(0.3)	16(15, 1) - 16(14, 2)	3ν ₁	[62023]
	8439.93	(0.10)	11(10, 1) - 10(9, 2)	2ν ₁	[62023]
	8450.16	(0.10)	11(10, 1) - 10(9, 2)	1ν ₁	[62023]
	8466.24	(0.10)	14(13, 1) - 14(12, 2)		[62023]
	8473.24	(0.10)	13(12, 1) - 13(12, 1)		[62023]
	8478.5	(0.3)	16(15, 1) - 16(14, 2)	4ν ₁	[62023]
	8483.8	(0.3)	11(10, 1) - 10(9, 2)	4ν ₁	[62023]
	8496.84	(0.3)	15(14, 1) - 15(13, 2)	2ν ₁	[62023]
	8510.47	(0.10)	15(14, 1) - 15(13, 2)		[62023]
	8524.64	(0.10)	12(11, 1) - 12(10, 2)		[62023]
	8558.23	(0.10)	10(9, 1) - 10(8, 2)	2ν ₁	[62023]
	8582.94	(0.10)	18(17, 1) - 18(16, 2)	1ν ₁	[62023]
	8596.76	(0.10)	10(9, 1) - 10(8, 2)	1ν ₁	[62023]
	8611.58	(0.10)	16(15, 1) - 16(14, 2)		[62023]
	8613.38	(0.10)	11(10, 1) - 11(9, 2)		[62023]
	8656.7	(0.3)	17(16, 1) - 17(15, 2)	4ν ₁	[62023]
	8683.31	(0.10)	16(15, 1) - 16(14, 2)	2ν ₁	[62023]
	8710.54	(0.10)	9(8, 1) - 9(7, 2)	2ν ₁	[62023]
	8732.39	(0.10)	10(9, 1) - 10(8, 2)		[62023]
	8762.50	(0.10)	9(8, 1) - 9(7, 2)	1ν ₁	[62023]
	8772.62	(0.10)	9(8, 1) - 9(7, 2)	4ν ₁	[62023]
	8775.04	(0.10)	17(16, 1) - 17(15, 2)		[62023]
	8787.73	(0.10)	9(8, 1) - 9(7, 2)	3ν ₁	[62023]
	8822.58	(0.10)	19(18, 1) - 19(17, 2)	1ν ₁	[62023]
	8824.66	(0.10)	18(17, 1) - 18(16, 2)	3ν ₁	[62023]
	8872.70	(0.10)	9(8, 1) - 9(7, 2)		[62023]
	8885.86	(0.10)	8(7, 1) - 8(6, 2)	2ν ₁	[62023]
	8907.3	(0.3)	18(17, 1) - 18(16, 2)	4ν ₁	[62023]
	8940.05	(0.10)	8(7, 1) - 8(6, 2)	1ν ₁	[62023]
	8944.65	(0.10)	8(7, 1) - 8(6, 2)	4ν ₁	[62023]
	8951.56	(0.10)	17(16, 1) - 17(15, 2)	2ν ₁	[62023]
	8958.59	(0.10)	8(7, 1) - 8(6, 2)	3ν ₁	[62023]
	9006.03	(0.10)	18(17, 1) - 18(16, 2)		[62023]
	9026.99	(0.10)	8(7, 1) - 8(6, 2)		[62023]
	9073.50	(0.10)	7(6, 1) - 7(5, 2)	2ν ₁	[62023]
	9115.08	(0.10)	20(19, 1) - 20(18, 2)	1ν ₁	[62023]
	9121.02	(0.10)	7(6, 1) - 7(5, 2)	1ν ₁	[62023]
	9123.23	(0.10)	7(6, 1) - 7(5, 2)	4ν ₁	[62023]
	9125.84	(0.10)	19(18, 1) - 19(17, 2)	3ν ₁	[62023]
	9134.72	(0.10)	7(6, 1) - 7(5, 2)	3ν ₁	[62023]
	9187.10	(0.10)	7(6, 1) - 7(5, 2)		[62023]
	9234.3	(0.3)	19(18, 1) - 19(17, 2)	4ν ₁	[62023]
	9263.29	(0.10)	6(5, 1) - 6(4, 2)	2ν ₁	[62023]
	9297.51	(0.10)	6(5, 1) - 6(4, 2)	1ν ₁	[62023]
	9299.71	(0.10)	6(5, 1) - 6(4, 2)	4ν ₁	[62023]
	9306.50	(0.10)	18(17, 1) - 18(16, 2)	2ν ₁	[62023]
	9308.08	(0.10)	6(5, 1) - 6(4, 2)	3ν ₁	[62023]
	9308.98	(0.10)	19(18, 1) - 19(17, 2)		[62023]
	9345.34	(0.10)	6(5, 1) - 6(4, 2)		[62023]
	9438.80	(0.10)	21(20, 1) - 21(19, 2)	1ν ₁	[62023]

TABLE 50.2. Microwave spectrum of cyclopentene — Continued

C₅H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	9445.08	(0.10)	5(4, 1) - 5(3, 2)	2ν ₁	[62023]
	9462.63	(0.10)	5(4, 1) - 5(3, 2)	1ν ₁	[62023]
	9466.26	(0.10)	5(4, 1) - 5(3, 2)	4ν ₁	[62023]
	9470.69	(0.10)	5(4, 1) - 5(3, 2)	3ν ₁	[62023]
	9495.06	(0.10)	5(4, 1) - 5(3, 2)		[62023]
	9503.9	(0.3)	20(19, 1) - 20(18, 2)	3ν ₁	[62023]
	9609.97	(0.10)	4(3, 1) - 4(2, 2)	1ν ₁	[62023]
	9610.38	(0.10)	4(3, 1) - 4(2, 2)	2ν ₁	[62023]
	9616.7	(0.3)	4(3, 1) - 4(2, 2)	3ν ₁	[62023]
	9629.52	(0.10)	4(3, 1) - 4(2, 2)		[62023]
	9641.5	(0.3)	20(19, 1) - 20(18, 2)	4ν ₁	[62023]
	9687.87	(0.10)	20(19, 1) - 20(18, 2)		[62023]
	9734.41	(0.10)	3(2, 1) - 3(1, 2)	1ν ₁	[62023]
	9740.28	(0.10)	3(2, 1) - 3(1, 2)	3ν ₁	[62023]
	9743.60	(0.10)	3(2, 1) - 3(2, 1)		[62023]
	9751.69	(0.10)	3(2, 1) - 3(1, 2)	2ν ₁	[62023]
	9752.52	(0.10)	19(18, 1) - 19(17, 2)	2ν ₁	[62023]
	9831.41	(0.10)	2(1, 1) - 2(0, 2)	1ν ₁	[62023]
	9833.07	(0.10)	2(1, 1) - 2(0, 2)		[62023]
	9862.77	(0.10)	2(1, 1) - 2(0, 2)	2ν ₁	[62023]
	9961.7	(0.3)	21(20, 1) - 21(19, 2)	3ν ₁	[62023]
	10028.43	(0.10)	2(2, 1) - 2(1, 2)	1ν ₁	[62023]
	10032.07	(0.10)	2(2, 1) - 2(2, 1)		[62023]
	10038.21	(0.10)	2(2, 1) - 2(1, 2)	3ν ₁	[62023]
	10096.68	(0.10)	2(2, 1) - 2(1, 2)	2ν ₁	[62023]
	10125.68	(0.10)	3(3, 1) - 3(2, 2)	1ν ₁	[62023]
	10131.65	(0.10)	21(20, 1) - 21(19, 2)	4ν ₁	[62023]
	10138.40	(0.10)	3(3, 1) - 3(2, 2)		[62023]
	10139.97	(0.10)	3(3, 1) - 3(2, 2)	3ν ₁	[62023]
	10145.88	(0.10)	21(20, 1) - 21(19, 2)		[62023]
	10215.16	(0.10)	3(3, 1) - 3(2, 2)	2ν ₁	[62023]
	10255.74	(0.10)	4(4, 1) - 4(3, 2)	1ν ₁	[62023]
	10275.99	(0.10)	4(4, 1) - 4(3, 2)	3ν ₁	[62023]
	10280.60	(0.10)	4(4, 1) - 4(3, 2)		[62023]
	10292.50	(0.10)	20(19, 1) - 20(18, 2)	2ν ₁	[62023]
	10295.40	(0.10)	4(4, 1) - 4(3, 2)	4ν ₁	[62023]
	10373.43	(0.10)	4(4, 1) - 4(3, 2)	2ν ₁	[62023]
	10419.15	(0.10)	5(5, 1) - 5(4, 2)	1ν ₁	[62023]
	10446.61	(0.10)	5(5, 1) - 5(4, 2)	3ν ₁	[62023]
	10458.67	(0.10)	5(5, 1) - 5(4, 2)		[62023]
	10471.44	(0.10)	5(5, 1) - 5(4, 2)	4ν ₁	[62023]
	10501.6	(0.3)	22(21, 1) - 22(20, 2)	3ν ₁	[62023]
	10572.38	(0.10)	5(5, 1) - 5(4, 2)	2ν ₁	[62023]
	10616.00	(0.10)	6(6, 1) - 6(5, 2)	1ν ₁	[62023]
	10652.12	(0.10)	6(6, 1) - 6(5, 2)	3ν ₁	[62023]
	10672.96	(0.10)	6(6, 1) - 6(5, 2)		[62023]
	10683.6	(0.3)	6(6, 1) - 6(5, 2)	4ν ₁	[62023]
	10684.93	(0.10)	22(21, 1) - 22(20, 2)		[62023]
	10706.1	(0.3)	22(21, 1) - 22(20, 2)	4ν ₁	[62023]
	10812.00	(0.10)	6(6, 1) - 6(5, 2)	2ν ₁	[62023]
	10846.59	(0.10)	7(7, 1) - 7(6, 2)	1ν ₁	[62023]
	10892.85	(0.10)	7(7, 1) - 7(6, 2)	3ν ₁	[62023]
	10923.90	(0.10)	7(7, 1) - 7(6, 2)		[62023]
	10932.02	(0.10)	7(7, 1) - 7(6, 2)	4ν ₁	[62023]
	11092.74	(0.10)	7(7, 1) - 7(6, 2)	2ν ₁	[62023]
	11111.57	(0.10)	8(8, 1) - 8(7, 2)	1ν ₁	[62023]
	11125.0	(0.3)	23(22, 1) - 23(21, 2)	3ν ₁	[62023]
	11169.08	(0.10)	8(8, 1) - 8(7, 2)	3ν ₁	[62023]
	11210.93	(0.10)	8(8, 1) - 8(7, 2)		[62023]
	11217.18	(0.10)	8(8, 1) - 8(7, 2)	4ν ₁	[62023]
	11242.92	(0.10)	1(1, 1) - 0(0, 0)		[62023]
	11244.98	(0.10)	1(1, 1) - 0(0, 0)	1ν ₁	[62023]
	11306.31	(0.10)	23(22, 1) - 23(22, 1)		[62023]
	11411.15	(0.10)	9(9, 1) - 9(8, 2)	1ν ₁	[62023]
	11415.10	(0.10)	8(8, 1) - 8(7, 2)	2ν ₁	[62023]
	11481.19	(0.10)	9(9, 1) - 9(8, 2)	3ν ₁	[62023]
	11535.02	(0.10)	9(9, 1) - 9(8, 2)		[62023]

TABLE 50.2. Microwave spectrum of cyclopentene — Continued

C₅H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	11539.42	(0.10)	9(9, 1) - 9(8, 2)	4ν ₁	[62023]
	11745.61	(0.10)	10(10, 1) - 10(9, 2)	1ν ₁	[62023]
	11779.34	(0.10)	9(9, 1) - 9(8, 2)	2ν ₁	[62023]
	11829.37	(0.10)	10(10, 1) - 10(9, 2)	3ν ₁	[62023]
	11895.80	(0.10)	10(10, 1) - 10(9, 2)		[62023]
	11898.44	(0.10)	10(10, 1) - 10(9, 2)	4ν ₁	[62023]
	12008.90	(0.10)	24(23, 1) - 24(22, 2)		[62023]
	12115.24	(0.10)	11(11, 1) - 11(10, 2)	1ν ₁	[62023]
	12185.58	(0.10)	10(10, 1) - 10(9, 2)	2ν ₁	[62023]
	12213.43	(0.10)	11(11, 1) - 11(10, 2)	3ν ₁	[62023]
	12293.54	(0.10)	11(11, 1) - 11(10, 2)		[62023]
	12294.98	(0.10)	11(11, 1) - 11(10, 2)	4ν ₁	[62023]
	12519.77	(0.10)	12(12, 1) - 12(11, 2)	1ν ₁	[62023]
	12633.75	(0.10)	12(12, 1) - 12(11, 2)	3ν ₁	[62023]
	12727.90	(0.10)	12(12, 1) - 12(12, 1)		[62023]
	12790.30	(0.10)	25(24, 1) - 25(23, 2)		[62023]
	12960.03	(0.10)	13(13, 1) - 13(12, 2)	1ν ₁	[62023]
	13089.93	(0.10)	13(13, 1) - 13(12, 2)	3ν ₁	[62023]
	13124.13	(0.10)	12(12, 1) - 12(11, 2)	2ν ₁	[62023]
	13198.7	(0.3)	13(13, 1) - 13(12, 2)		[62023]
	13434.97	(0.10)	14(14, 1) - 14(13, 2)	1ν ₁	[62023]
	13581.78	(0.10)	14(14, 1) - 14(13, 2)	3ν ₁	[62023]
	13656.2	(0.3)	13(13, 1) - 13(12, 2)	2ν ₁	[62023]
	13705.1	(0.3)	14(14, 1) - 14(13, 2)		[62023]
	13706.6	(0.3)	14(14, 1) - 14(13, 2)	4ν ₁	[62023]
	13944.1	(0.3)	15(15, 1) - 15(14, 2)	1ν ₁	[62023]
	14108.7	(0.3)	15(15, 1) - 15(14, 2)	3ν ₁	[62023]
	14228.7	(0.3)	14(14, 1) - 14(13, 2)	2ν ₁	[62023]
	14246.2	(0.3)	15(15, 1) - 15(14, 2)		[62023]
	14487.50	(0.10)	16(16, 1) - 16(15, 2)	1ν ₁	[62023]
	14670.75	(0.10)	16(16, 1) - 16(15, 2)	3ν ₁	[62023]
	14820.90	(0.10)	16(16, 1) - 16(15, 2)		[62023]
	14828.7	(0.3)	16(16, 1) - 16(15, 2)	4ν ₁	[62023]
	14841.1	(0.3)	15(15, 1) - 15(14, 2)	2ν ₁	[62023]
	15063.75	(0.10)	17(17, 1) - 17(16, 2)	1ν ₁	[62023]
	16324.8	(0.2)	9(7, 2) - 9(6, 3)	2ν ₁	[65035]
	16329.6	(0.2)	9(7, 2) - 9(6, 3)	4ν ₁	[65035]
	16409.7	(0.2)	8(6, 2) - 8(5, 3)	3ν ₁	[65035]
	16415.9	(0.2)	8(6, 2) - 8(5, 3)	4ν ₁	[65035]
	16431.8	(0.2)	8(6, 2) - 8(5, 3)	2ν ₁	[65035]
	16468.73	(0.20)	7(5, 2) - 7(4, 3)	3ν ₁	[65035]
	16478.10	(0.20)	7(5, 2) - 7(4, 3)	4ν ₁	[65035]
	16509.25	(0.20)	6(4, 2) - 6(3, 3)	3ν ₁	[65035]
	16520.45	(0.20)	6(4, 2) - 6(3, 3)	4ν ₁	[65035]
	16527.03	(0.20)	7(5, 2) - 7(4, 3)	2ν ₁	[65035]
	16534.53	(0.20)	5(3, 2) - 5(2, 3)	3ν ₁	[65035]
	16557.05	(0.20)	3(1, 2) - 3(0, 3)	3ν ₁	[65035]
	16562.28	(0.20)	6(4, 2) - 6(3, 3)	2ν ₁	[65035]
	16563.15	(0.20)	3(2, 2) - 3(1, 3)	3ν ₁	[65035]
	16564.88	(0.20)	4(3, 2) - 4(2, 3)	3ν ₁	[65035]
	16570.40	(0.20)	5(4, 2) - 5(3, 3)	3ν ₁	[65035]
	16580.10	(0.20)	6(3, 2) - 6(4, 3)	3ν ₁	[65035]
	16595.8	(0.2)	7(6, 2) - 7(5, 3)	3ν ₁	[65035]
	16596.10	(0.20)	5(3, 2) - 5(2, 3)	2ν ₁	[65035]
	16612.9	(0.2)	7(6, 2) - 7(5, 3)	4ν ₁	[65035]
	16615.78	(0.20)	4(2, 2) - 4(1, 3)	2ν ₁	[65035]
	16625.68	(0.20)	3(1, 2) - 3(0, 3)	2ν ₁	[65035]
	16632.95	(0.20)	3(2, 2) - 3(1, 3)	2ν ₁	[65035]
	16636.48	(0.20)	4(3, 2) - 4(2, 3)	2ν ₁	[65035]
	16644.20	(0.20)	5(4, 2) - 5(3, 3)	2ν ₁	[65035]
	16657.68	(0.20)	6(5, 2) - 5(4, 3)	2ν ₁	[65035]
	16679.2	(0.2)	7(6, 2) - 7(5, 3)	2ν ₁	[65035]
	18948.8	(0.2)	2(0, 2) - 1(1, 1)	2ν ₁	[65035]
	19028.70	(0.20)	2(1, 2) - 1(0, 1)	2ν ₁	[65035]
	19036.35	(0.20)	2(0, 2) - 1(1, 1)	3ν ₁	[65035]
	19073.50	(0.10)	2(0, 2) - 1(1, 1)		[62023]
	19080.86	(0.10)	2(0, 2) - 1(1, 1)	1ν ₁	[62023]

TABLE 50.2. Microwave spectrum of cyclopentene — Continued

C₅H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	19105.05	(0.20)	2(1, 2) - 1(0, 1)	3ν ₁	[65035]
	19141.32	(0.10)	2(1, 2) - 1(0, 1)		[62023]
	19148.14	(0.10)	2(1, 2) - 1(0, 1)	1ν ₁	[62023]
	25759.73	(0.20)	2(2, 1) - 1(1, 0)	2ν ₁	[65035]
	25797.2	(0.2)	2(2, 1) - 1(1, 0)	3ν ₁	[65035]
	25829.15	(0.10)	2(2, 1) - 1(1, 0)		[62023]
	25833.62	(0.10)	2(2, 1) - 1(1, 0)	1ν ₁	[62023]
	27005.21	(0.10)	3(0, 3) - 2(2, 1)		[62023]
	27006.20	(0.10)	3(1, 3) - 2(0, 2)		[62023]
	27021.21	(0.10)	3(0, 3) - 2(1, 2)	1ν ₁	[62023]
	27022.10	(0.10)	3(1, 3) - 2(0, 2)	1ν ₁	[62023]
	32319.29	(0.10)	2(2, 0) - 1(1, 1)		[62023]
	32321.94	(0.10)	2(2, 0) - 1(1, 1)	1ν ₁	[62023]
	33516.77	(0.10)	3(1, 2) - 2(2, 1)		[62023]
	33535.80	(0.10)	3(1, 2) - 2(2, 1)	1ν ₁	[62023]
	33722.08	(0.10)	3(2, 2) - 2(1, 1)		[62023]
	33738.68	(0.10)	3(2, 2) - 2(1, 1)	1ν ₁	[62023]

Table 51.1. Molecular constants of
1,1-dimethylcyclopropane,
 $(\text{CH}_3)_2\overset{\text{C}}{\text{C}}\text{CH}_2\text{CH}_2$.

Parameter	Value
A'' (MHz)	6135.2636(414)
B'' (MHz)	5203.3487(393)
C'' (MHz)	3810.597(48)
τ ₁ (kHz)	-39.601(16061)
τ ₂ (kHz)	-13.044(5355)
τ ₃ ^a (kHz)	504.1(1182)
τ _{aaaa} (kHz)	-21.31(568)
τ _{bbbb} (kHz)	-16.58(541)
τ _{cccc} (kHz)	-21.67(574)
μ _a (D)	0.142(1) [79031]

^aValue fixed by setting R_g = 0.

TABLE 51.2. Microwave spectrum of 1,1-dimethylcyclopropane

C₅H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
C(CH ₃) ₂ CH ₂ CH ₂	26616.25	(0.05)	9(3, 7) - 9(1, 8)	[79031]
	27041.24	(0.05)	3(2, 2) - 2(2, 1)	[79031]
	27548.18	(0.05)	14(9, 6) - 14(7, 7)	[79031]
	28373.19	(0.05)	3(1, 2) - 2(1, 1)	[79031]
$ \begin{array}{c} \text{H}_2\text{C}-\text{CH}_2 \\ \diagdown \quad / \\ \text{C} \\ / \quad \diagdown \\ \text{CH}_3 \quad \text{CH}_3 \end{array} $	28416.50	(0.05)	11(8, 4) - 11(6, 5)	[79031]
	29289.76	(0.05)	3(2, 1) - 2(2, 0)	[79031]
	29769.34	(0.05)	16(10, 7) - 16(8, 8)	[79031]
	30700.22	(0.05)	13(9, 5) - 13(7, 6)	[79031]
	31958.89	(0.05)	18(11, 8) - 18(9, 9)	[79031]
	32255.26	(0.05)	4(1, 4) - 3(1, 3)	[79031]
	32320.48	(0.05)	4(0, 4) - 3(0, 3)	[79031]
	32785.56	(0.05)	15(10, 6) - 15(8, 7)	[79031]
	34146.74	(0.05)	20(12, 9) - 20(10, 10)	[79031]
	35358.74	(0.05)	12(9, 4) - 12(7, 5)	[79031]
	35382.89	(0.05)	4(2, 3) - 3(2, 2)	[79031]
	36080.51	(0.05)	16(7, 10) - 16(5, 11)	[79031]
	36324.90	(0.05)	4(1, 3) - 3(1, 2)	[79031]
	37068.63	(0.05)	4(3, 2) - 3(3, 1)	[79031]

Table 52.1. Molecular constants of the ground state of trans-3-methyl-1-butene.

Parameter	Value
A'' (MHz)	7536.35(11)
B'' (MHz)	3550.9907(102)
C'' (MHz)	2741.6525(113)
τ_1 (kHz)	-88.75(41)
τ_2 (kHz)	-18.86(41)
τ_3^a (kHz)	0.295(33)
τ_{aaaa} (kHz)	0 ^b
τ_{bbbb} (kHz)	-3.89(69)
τ_{cccc} (kHz)	-0.98(72)
μ_a (D)	0.312(3) [79032]
μ_c (D)	0.071(42) [79032]

^aValue fixed by setting $R_6 = 0$.^bFixed at zero.

Table 52.2. Molecular constants of the vibrational states of trans-3-methyl-1-butene. [79032]

Parameter	$\nu_{39} = 1$	$\nu_{39} = 2$	$\nu_{39} = 3$
A (MHz)	7536.561(368) ^a	7536.938(256)	7536.950(250)
B (MHz)	3567.316(30)	3583.788(21)	3600.419(22)
C (MHz)	2742.475(30)	2743.243(22)	2743.938(22)
Δ_J (kHz)	0.5(2)	0.6(1)	0.8(2)
Δ_{JK} (kHz)	21.4(8)	22.2(6)	22.9(7)
Δ_K (kHz)	-43.2(1030)	-13.5(683)	5.1(638)
δ_J (kHz)	0.2(2)	0.2(1)	0.1(1)
δ_K (kHz)	6.4(66)	---	12.3(47)

^aUncertainties quoted here are two times the standard deviation.

Table 52.3. Molecular constants for gauche-3-methyl-1-butene.

Parameter	Ground State ^a	$\nu_{39} = 1^d$	$\nu_{39} = 2^d$
A'' (MHz)	7294.185(37)	7280.47(50)	7268.91(56)
B'' (MHz)	3916.1226(48)	3914.90(2)	3913.03(3)
C'' (MHz)	2879.3045(45)	2883.36(2)	2887.03(2)
τ_1 (kHz)	-17.99(50)		
τ_2 (kHz)	-5.05(19)		
τ_3^b (kHz)	130.(20)		
τ_{aaaa} (kHz)	0 ^c		
τ_{bbbb} (kHz)	-5.96(47)		
τ_{cccc} (kHz)	-3.47(27)		
μ_a (D)	0.367(4)		
μ_c (D)	0.154(6)		
E_g (cm ⁻¹)	129.5 ^e		

^aPresent work.

^bValue fixed by setting $R_g = 0$.

^cFixed at zero.

^dValues from [79032]. Uncertainties are two standard deviations.

^eWith respect to the trans isomer.

TABLE 52.4. Microwave spectrum of 3-methyl-1-butene

C₅H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
<i>t</i> -CH ₂ CHCH(CH ₃) ₂	26535.23	(0.02)	4(1, 3) - 3(1, 2)		[79032]
	29042.59	(0.02)	5(1, 5) - 4(1, 4)		[79032]
	29679.94	(0.02)	5(0, 5) - 4(0, 4)		[79032]
	31215.37	(0.02)	5(2, 4) - 4(2, 3)		[79032]
	31706.00	(0.02)	5(4, 2) - 4(4, 1)		[79032]
	31711.42	(0.02)	5(4, 1) - 4(4, 0)		[79032]
	31752.54	(0.02)	5(3, 3) - 4(3, 2)		[79032]
	31947.35	(0.02)	5(3, 2) - 4(3, 1)		[79032]
	32992.60	(0.02)	5(2, 3) - 4(2, 2)		[79032]
	34666.80	(0.02)	6(1, 6) - 5(1, 5)		[79032]
	35096.88	(0.02)	6(0, 6) - 5(0, 5)		[79032]
	37260.57	(0.02)	6(2, 5) - 5(2, 4)		[79032]
	38028.91	(0.02)	6(5, 2) - 5(5, 1)		[79032]
	38029.23	(0.02)	6(5, 1) - 5(5, 0)		[79032]
	38121.61	(0.02)	6(4, 3) - 5(4, 2)		[79032]
	38133.16	(0.02)	6(3, 4) - 5(3, 3)		[79032]
	38146.03	(0.02)	6(4, 2) - 5(4, 1)		[79032]
	38626.20	(0.02)	6(3, 3) - 5(3, 2)		[79032]
	39029.03	(0.02)	6(1, 5) - 5(1, 4)		[79032]
	39894.36	(0.02)	6(2, 4) - 5(2, 3)		[79032]
	26624.02	(0.02)	4(1, 3) - 3(1, 2)		1ν ₃₉ [79032]
	29075.52	(0.02)	5(1, 5) - 4(1, 4)		1ν ₃₉ [79032]
	29707.48	(0.02)	5(0, 5) - 4(0, 4)		1ν ₃₉ [79032]
	31291.37	(0.02)	5(2, 4) - 4(2, 3)		1ν ₃₉ [79032]
	31801.75	(0.02)	5(4, 2) - 4(4, 1)		1ν ₃₉ [79032]
	31807.66	(0.02)	5(4, 1) - 4(4, 0)		1ν ₃₉ [79032]
	31848.46	(0.02)	5(3, 3) - 4(3, 2)		1ν ₃₉ [79032]
	32055.08	(0.02)	5(3, 2) - 4(3, 1)		1ν ₃₉ [79032]
	32992.71	(0.02)	5(1, 4) - 4(1, 3)		1ν ₃₉ [79032]
	33126.58	(0.02)	5(2, 3) - 4(2, 2)		1ν ₃₉ [79032]
	34700.91	(0.02)	6(1, 6) - 5(1, 5)		1ν ₃₉ [79032]
	35122.38	(0.02)	6(0, 6) - 5(0, 5)		1ν ₃₉ [79032]
	37344.00	(0.02)	6(2, 5) - 5(2, 4)		1ν ₃₉ [79032]
	38143.20	(0.02)	6(5, 2) - 5(5, 1)		1ν ₃₉ [79032]
	38143.60	(0.02)	6(5, 1) - 5(5, 0)		1ν ₃₉ [79032]
	38239.24	(0.02)	6(4, 3) - 5(4, 2)		1ν ₃₉ [79032]
	38247.42	(0.02)	6(3, 4) - 5(3, 3)		1ν ₃₉ [79032]
	38265.70	(0.02)	6(4, 2) - 5(4, 1)		1ν ₃₉ [79032]
	38769.10	(0.02)	6(3, 3) - 5(3, 2)		1ν ₃₉ [79032]
	39127.38	(0.02)	6(1, 5) - 5(1, 4)		1ν ₃₉ [79032]
	26712.90	(0.02)	4(1, 3) - 3(1, 2)		2ν ₃₉ [79032]
	29107.78	(0.02)	5(1, 5) - 4(1, 4)		2ν ₃₉ [79032]
	29734.00	(0.02)	5(0, 5) - 4(0, 4)		2ν ₃₉ [79032]
	31367.23	(0.02)	5(2, 4) - 4(2, 3)		2ν ₃₉ [79032]
	31898.04	(0.02)	5(4, 2) - 4(4, 1)		2ν ₃₉ [79032]
	31904.44	(0.02)	5(4, 1) - 4(4, 0)		2ν ₃₉ [79032]
	31944.81	(0.02)	5(3, 3) - 4(3, 2)		2ν ₃₉ [79032]
	32163.86	(0.02)	5(3, 2) - 4(3, 1)		2ν ₃₉ [79032]
	33091.02	(0.02)	5(1, 4) - 4(1, 3)		2ν ₃₉ [79032]
	33261.57	(0.02)	5(2, 3) - 4(2, 2)		2ν ₃₉ [79032]
	34734.13	(0.02)	6(1, 6) - 5(1, 5)		2ν ₃₉ [79032]
	35146.86	(0.02)	6(0, 6) - 5(0, 5)		2ν ₃₉ [79032]
	37427.09	(0.02)	6(2, 5) - 5(2, 4)		2ν ₃₉ [79032]
	38258.06	(0.02)	6(5, 2) - 5(5, 1)		2ν ₃₉ [79032]
	38258.55	(0.02)	6(5, 1) - 5(5, 0)		2ν ₃₉ [79032]
	38357.53	(0.02)	6(4, 3) - 5(4, 2)		2ν ₃₉ [79032]
	38362.02	(0.02)	6(3, 4) - 5(3, 3)		2ν ₃₉ [79032]
	38386.19	(0.02)	6(4, 2) - 5(4, 1)		2ν ₃₉ [79032]
	38913.74	(0.02)	6(3, 3) - 5(3, 2)		2ν ₃₉ [79032]
	39224.55	(0.02)	6(1, 5) - 5(1, 4)		2ν ₃₉ [79032]
	26802.21	(0.02)	4(1, 3) - 3(1, 2)		3ν ₃₉ [79032]
	29139.36	(0.02)	5(1, 5) - 4(1, 4)		3ν ₃₉ [79032]
	29759.49	(0.02)	5(0, 5) - 4(0, 4)		3ν ₃₉ [79032]
	31443.15	(0.02)	5(2, 4) - 4(2, 3)		3ν ₃₉ [79032]
31995.07	(0.02)	5(4, 2) - 4(4, 1)		3ν ₃₉ [79032]	
32002.04	(0.02)	5(4, 1) - 4(4, 0)		3ν ₃₉ [79032]	
32041.91	(0.02)	5(3, 3) - 4(3, 2)		3ν ₃₉ [79032]	

TABLE 52.4. Microwave spectrum of 3-methyl-1-butene — Continued

C₅H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.	
<i>g</i> -CH ₂ CHCH(CH ₃) ₂	32274.09	(0.02)	5(3, 2) - 4(3, 1)	3ν ₃₉	[79032]	
	33189.15	(0.02)	5(1, 4) - 4(1, 3)	3ν ₃₉	[79032]	
	33398.00	(0.02)	5(2, 3) - 4(2, 2)	3ν ₃₉	[79032]	
	34766.37	(0.02)	6(1, 6) - 5(1, 5)	3ν ₃₉	[79032]	
	35170.25	(0.02)	6(0, 6) - 5(0, 5)	3ν ₃₉	[79032]	
	37509.95	(0.02)	6(2, 5) - 5(2, 4)	3ν ₃₉	[79032]	
	38373.82	(0.02)	6(5, 2) - 5(5, 1)	3ν ₃₉	[79032]	
	38374.34	(0.02)	6(5, 1) - 5(5, 0)	3ν ₃₉	[79032]	
	38476.86	(0.02)	6(4, 3) - 5(4, 2)	3ν ₃₉	[79032]	
	38477.44	(0.02)	6(3, 4) - 5(3, 3)	3ν ₃₉	[79032]	
	38507.90	(0.02)	6(4, 2) - 5(4, 1)	3ν ₃₉	[79032]	
	39060.72	(0.02)	6(3, 3) - 5(3, 2)	3ν ₃₉	[79032]	
	39320.81	(0.02)	6(1, 5) - 5(1, 4)	3ν ₃₉	[79032]	
	27020.98	(0.02)	4(2, 3) - 3(2, 2)			[79032]
	27524.00	(0.02)	4(3, 2) - 3(3, 1)			[79032]
	27674.28	(0.02)	4(3, 1) - 3(3, 0)			[79032]
	28711.64	(0.02)	4(2, 2) - 3(2, 1)			[79032]
	28762.00	(0.02)	4(1, 3) - 3(1, 2)			[79032]
	30714.61	(0.02)	5(1, 5) - 4(1, 4)			[79032]
	31172.26	(0.02)	5(0, 5) - 4(0, 4)			[79032]
	33524.21	(0.02)	5(2, 4) - 4(2, 3)			[79032]
	34428.64	(0.02)	5(4, 2) - 4(4, 1)			[79032]
	34449.67	(0.02)	5(4, 1) - 4(4, 0)			[79032]
	34451.64	(0.02)	5(3, 3) - 4(3, 2)			[79032]
	34947.13	(0.02)	5(3, 2) - 4(3, 1)			[79032]
	35402.81	(0.02)	5(1, 4) - 4(1, 3)			[79032]
	36307.39	(0.02)	5(2, 3) - 4(2, 2)			[79032]
	36584.74	(0.02)	6(1, 6) - 5(1, 5)			[79032]
	36831.20	(0.02)	6(0, 6) - 5(0, 5)			[79032]
	39876.56	(0.02)	6(2, 5) - 5(2, 4)			[79032]
	27033.91	(0.02)	4(2, 3) - 3(2, 2)		1ν ₃₉	[79032]
	27533.84	(0.02)	4(3, 2) - 3(3, 1)		1ν ₃₉	[79032]
	27682.96	(0.02)	4(3, 1) - 3(3, 0)		1ν ₃₉	[79032]
	28714.60	(0.02)	4(2, 2) - 3(2, 1)		1ν ₃₉	[79032]
	28766.47	(0.02)	4(1, 3) - 3(1, 2)		1ν ₃₉	[79032]
	30746.67	(0.02)	5(1, 5) - 4(1, 4)		1ν ₃₉	[79032]
	31202.96	(0.02)	5(0, 5) - 4(0, 4)		1ν ₃₉	[79032]
	33541.87	(0.02)	5(2, 4) - 4(2, 3)		1ν ₃₉	[79032]
	34440.68	(0.02)	5(4, 2) - 4(4, 1)		1ν ₃₉	[79032]
	34461.54	(0.02)	5(4, 1) - 4(4, 0)		1ν ₃₉	[79032]
	34463.78	(0.02)	5(3, 3) - 4(3, 2)		1ν ₃₉	[79032]
	34955.68	(0.02)	5(3, 2) - 4(3, 1)		1ν ₃₉	[79032]
	35411.97	(0.02)	5(1, 4) - 4(1, 3)		1ν ₃₉	[79032]
	36309.40	(0.02)	5(2, 3) - 4(2, 2)		1ν ₃₉	[79032]
	36624.67	(0.02)	6(1, 6) - 5(1, 5)		1ν ₃₉	[79032]
	36870.59	(0.02)	6(0, 6) - 5(0, 5)		1ν ₃₉	[79032]
	39899.88	(0.02)	6(2, 5) - 5(2, 4)		1ν ₃₉	[79032]
	27042.20	(0.02)	4(2, 3) - 3(2, 2)		2ν ₃₉	[79032]
27538.55	(0.02)	4(3, 2) - 3(3, 1)		2ν ₃₉	[79032]	
27686.31	(0.02)	4(3, 1) - 3(3, 0)		2ν ₃₉	[79032]	
30774.07	(0.02)	5(1, 5) - 4(1, 4)		2ν ₃₉	[79032]	
31229.71	(0.02)	5(0, 5) - 4(0, 4)		2ν ₃₉	[79032]	
33554.17	(0.02)	5(2, 4) - 4(2, 3)		2ν ₃₉	[79032]	
34446.25	(0.02)	5(4, 2) - 4(4, 1)		2ν ₃₉	[79032]	
34466.89	(0.02)	5(4, 1) - 4(4, 0)		2ν ₃₉	[79032]	
34469.56	(0.02)	5(3, 3) - 4(3, 2)		2ν ₃₉	[79032]	
34956.94	(0.02)	5(3, 2) - 4(3, 1)		2ν ₃₉	[79032]	
35416.17	(0.02)	5(1, 4) - 4(1, 3)		2ν ₃₉	[79032]	
36304.14	(0.02)	5(2, 3) - 4(2, 2)		2ν ₃₉	[79032]	
36659.16	(0.02)	6(1, 6) - 5(1, 5)		2ν ₃₉	[79032]	
36905.07	(0.02)	6(0, 6) - 5(0, 6)		2ν ₃₉	[79032]	
39917.12	(0.02)	6(2, 5) - 5(2, 4)		2ν ₃₉	[79032]	

Table 53.1. Molecular parameters of cis-2-pentene.

Parameter	A-species (Eq. 4) ^a	Parameter	General Hamiltonian (Eq. 1) ^a
A (MHz)	10987.805(41)		10985.103(50)
B (MHz)	2601.395(5)		2600.896(10)
C (MHz)	2371.405(5)		2371.299(11)
Δ_J (kHz)	4.72(4)		4.71(3)
Δ_{JK} (kHz)	-81.2(2)		-81.8(2)
Δ_K (kHz)	478.(13)		478.(8)
δ_J (kHz)	0.569(2)		0.560(2)
δ_K (kHz)	-41.1(3)		-42.0(2)
H_J (Hz)	-0.6(1)	ρ_a	0.03349(12)
H_{JK} (Hz)	-5.0(9)	ρ_b	0.01430(4)
H_{KJ} (Hz)	122.(42)	ρ_c	0.00125(8)
H_K (Hz)	-1800.(1200)	V_3 (cm^{-1})	277.(1)
h_J (Hz)	0.036(5)	I_α ($\text{u } \text{Å}^2$)	3.189(10)
h_{JK} (Hz)	-0.5(9)	s	22.649(16)
h_K (Hz)	-43.(33)	F (GHz)	163.2(5)
<u>Electric Dipole Moment</u>			
μ_a (D)	0.002(2)		
μ_b (D)	0.274(3)		
μ_c (D)	0.070(12)		

^aSee reference [81037].

Table 53.2. Molecular parameters of excited torsional states of cis-2-pentene. [81037]

Parameter	v = 1	v = 2
A (MHz)	10868.956(53)	10811.562(38)
B (MHz)	2637.681(10)	2670.390(8)
C (MHz)	2396.975(10)	2417.859(8)
Δ_J (kHz)	6.74(3)	7.74(3)
Δ_{JK} (kHz)	-107.2(2)	-115.0(1)
Δ_K (kHz)	567.(7)	581.(5)
δ_J (kHz)	1.063(2)	1.453(1)
δ_K (kHz)	-55.1(2)	-56.5(1)
H_{JK} (Hz)	-6.1(7)	-3.3(4)
h_J (Hz)	0.085(8)	0.081(6)
h_{JK} (Hz)	0.2(11)	5.5(7)
ρ_a	0.03528(11)	0.03884(7)
ρ_b	0.01478(4)	0.01543(2)
ρ_c	0.00184(4)	0.00252(2)
I_α (u \AA^2)	3.295 (Eq. 4)	3.479 (Eq. 4)
	3.189 (fixed)	3.189 (fixed)
V_3 (cm^{-1})	272.(1) (Eq. 4)	264.(1) (Eq. 4)
	284.(1) (fixed)	295.(1) (fixed)
$\sigma_{\bar{\nu}}^a$ (MHz)	0.23	0.13
ΔE (MHz)	1.2(1)	18.6(1)
α		-4.6° (assumed)
β	22.8(5)°	24.9(1)°
γ	3.4(7)°	3.5(1)°
ΔR_{xx} (kHz)		260.(7)
ΔR_{yy} (kHz)		-8.4(8)
ΔR_{zz} (kHz)		-24.4(3)
ΔR_{xy} (kHz)		3.7(9)
$\sigma_{\Delta\nu}^a$ (MHz)	0.03	0.06

^a $\sigma_{\bar{\nu}}$ and $\sigma_{\Delta\nu}$ give the r.m.s. deviations of the average frequencies and the doublet splittings, respectively. For further explanation see [81037].

TABLE 53.3. Microwave spectrum of 2-pentene

C₅H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-i}, K_{-i}) - J''(K_{+i}, K_{+i})$	V_i	Sym.	Ref.
c-CH ₃ CHCHCH ₂ CH ₃	22001.40	(0.10)	9(2, 7) - 9(1, 8)	0	A	[81037]
	22009.00	(0.10)	9(2, 7) - 9(1, 8)	0	E	[81037]
	22211.49	(0.10)	15(2, 13) - 15(1, 14)	1	E	[81037]
	22231.11	(0.10)	15(2, 13) - 15(1, 14)	1	A	[81037]
	22250.93	(0.10)	15(2, 13) - 15(1, 14)	0	A	[81037]
	22268.40	(0.10)	15(2, 13) - 15(1, 14)	0	E	[81037]
	22440.86	(0.10)	8(2, 6) - 8(1, 7)	0	A	[81037]
	22454.78	(0.10)	8(2, 6) - 8(1, 7)	0	E	[81037]
	22692.32	(0.10)	13(1, 12) - 13(0, 13)	0	E	[81037]
	22748.40	(0.10)	13(1, 12) - 13(0, 13)	0	A	[81037]
	23004.85	(0.10)	16(2, 14) - 16(1, 15)	0	E	[81037]
	23029.15	(0.10)	16(2, 14) - 16(1, 15)	0	A	[81037]
	23104.73	(0.10)	16(2, 14) - 16(1, 15)	1	E	[81037]
	23131.22	(0.10)	16(2, 14) - 16(1, 15)	1	A	[81037]
	24011.15	(0.10)	17(2, 15) - 17(1, 16)	0	E	[81037]
	24043.52	(0.10)	17(2, 15) - 17(1, 16)	0	A	[81037]
	24267.61	(0.10)	17(2, 15) - 17(1, 16)	1	E	[81037]
	24302.35	(0.10)	17(2, 15) - 17(1, 16)	1	A	[81037]
	25238.41	(0.10)	14(1, 13) - 14(0, 14)	0	E	[81037]
	25303.68	(0.10)	14(1, 13) - 14(0, 14)	0	A	[81037]
	25281.76	(0.10)	18(2, 16) - 18(1, 17)	0	E	[81037]
	25323.35	(0.10)	18(2, 16) - 18(1, 17)	0	A	[81037]
	25710.50	(0.10)	18(2, 16) - 18(1, 17)	1	E	[81037]
	25754.54	(0.10)	18(2, 16) - 18(1, 17)	1	A	[81037]
	26040.09	(0.10)	14(1, 13) - 14(0, 14)	1	E	[81037]
	26103.77	(0.10)	14(1, 13) - 14(0, 14)	1	A	[81037]
	26824.83	(0.10)	19(2, 17) - 19(1, 18)	0	E	[81037]
	26876.90	(0.10)	19(2, 17) - 19(1, 18)	0	A	[81037]
	26891.83	(0.10)	5(2, 4) - 5(1, 5)	1	A	[81037]
	27153.83	(0.10)	5(2, 4) - 5(1, 5)	0	E	[81037]
	27247.75	(0.10)	5(2, 4) - 5(1, 5)	0	A	[81037]
	27439.14	(0.10)	19(2, 17) - 19(1, 18)	1	E	[81037]
	27493.52	(0.10)	19(2, 17) - 19(1, 18)	1	A	[81037]
	27955.29	(0.10)	6(2, 5) - 6(1, 6)	0	A	[81037]
	27976.71	(0.10)	15(1, 14) - 15(0, 15)	0	E	[81037]
	28051.19	(0.10)	15(1, 14) - 15(0, 15)	0	A	[81037]
	28195.26	(0.10)	7(0, 7) - 6(1, 6)	0	E	[81037]
	28202.58	(0.10)	7(0, 7) - 6(1, 6)	0	A	[81037]
	28643.96	(0.10)	20(2, 18) - 20(1, 19)	0	E	[81037]
	28707.44	(0.10)	20(2, 18) - 20(1, 19)	0	A	[81037]
	28724.51	(0.10)	15(2, 14) - 14(3, 11)	0	E	[81037]
	28733.14	(0.10)	7(2, 6) - 7(1, 7)	0	E	[81037]
	28750.99	(0.10)	15(2, 14) - 14(3, 11)	0	A	[81037]
	28784.67	(0.10)	7(2, 6) - 7(1, 7)	0	A	[81037]
	28833.40	(0.10)	7(0, 7) - 6(1, 6)	1	E	[81037]
	28840.41	(0.10)	7(0, 7) - 6(1, 6)	1	A	[81037]
	28898.47	(0.10)	15(1, 14) - 15(0, 15)	1	E	[81037]
	28970.22	(0.10)	15(1, 14) - 15(0, 15)	1	A	[81037]
	29465.21	(0.10)	8(2, 7) - 8(1, 8)	1	E	[81037]
	29453.38	(0.10)	20(2, 18) - 20(1, 19)	1	E	[81037]
	29505.53	(0.10)	8(2, 7) - 8(1, 8)	1	A	[81037]
	29518.91	(0.10)	20(2, 18) - 20(1, 19)	1	A	[81037]
	29693.71	(0.10)	8(2, 7) - 8(1, 8)	0	E	[81037]
	29736.83	(0.10)	8(2, 7) - 8(1, 8)	0	A	[81037]
	30125.39	(0.10)	10(1, 9) - 9(2, 8)	0	E	[81037]
	30128.26	(0.10)	10(1, 9) - 9(2, 8)	0	A	[81037]
	30354.33	(0.10)	18(3, 16) - 18(2, 16)	1	A	[81037]
	30371.92	(0.10)	18(3, 16) - 18(2, 16)	1	E	[81037]
	30736.92	(0.10)	21(2, 19) - 21(1, 20)	0	E	[81037]
	30812.48	(0.10)	21(2, 19) - 21(1, 20)	0	A	[81037]
	30880.55	(0.10)	16(1, 15) - 16(0, 16)	0	E	[81037]
	30963.94	(0.10)	16(1, 15) - 16(0, 16)	0	A	[81037]
	31674.33	(0.10)	5(1, 5) - 4(0, 4)	0	E	[81037]
	31677.39	(0.10)	5(1, 5) - 4(0, 4)	0	A	[81037]
	31746.02	(0.10)	21(2, 19) - 21(1, 20)	1	E	[81037]
	31760.33	(0.10)	5(1, 5) - 4(0, 4)	1	E	[81037]
	31763.44	(0.10)	5(1, 5) - 4(0, 4)	1	A	[81037]
	31823.24	(0.10)	21(2, 19) - 21(1, 20)	1	A	[81037]

TABLE 53.3. Microwave spectrum of 2-pentene — Continued

C₅H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_-,K_-)$ - $J''(K_+,K_+)$	V_t	Sym.	Ref.
	31842.47	(0.10)	18(3,16) - 18(2,16)	0	A	[81037]
	31858.85	(0.10)	18(3,16) - 18(2,16)	0	E	[81037]
	31913.42	(0.10)	16(1,15) - 16(0,16)	1	E	[81037]
	31971.89	(0.10)	10(2, 9) - 10(1,10)	0	E	[81037]
	31993.02	(0.10)	16(1,15) - 16(0,16)	1	A	[81037]
	32012.00	(0.10)	10(2, 9) - 10(1,10)	0	A	[81037]
	32023.03	(0.10)	22(3,19) - 22(2,20)	1	E	[81037]
	32029.49	(0.10)	22(3,19) - 22(2,20)	1	A	[81037]
	32035.15	(0.10)	17(3,15) - 17(2,15)	1	A	[81037]
	32043.07	(0.10)	17(3,15) - 17(2,15)	1	E	[81037]
	32168.86	(0.10)	23(3,20) - 23(2,21)	1	E	[81037]
	32182.99	(0.10)	23(3,20) - 23(2,21)	1	A	[81037]
	32208.92	(0.10)	14(2,12) - 13(3,11)	0	A	[81037]
	32265.91	(0.10)	14(2,12) - 13(3,11)	0	E	[81037]
	32460.14	(0.10)	20(3,17) - 20(2,18)	1	A	[81037]
	32465.28	(0.10)	20(3,17) - 20(2,18)	1	E	[81037]
	32563.66	(0.10)	23(3,20) - 23(2,21)	0	E	[81037]
	32571.70	(0.10)	23(3,20) - 23(2,21)	0	A	[81037]
	32590.92	(0.10)	24(3,21) - 24(2,22)	1	E	[81037]
	32598.34	(0.10)	22(3,19) - 22(2,20)	0	E	[81037]
	32599.05	(0.10)	22(3,19) - 22(2,20)	0	A	[81037]
	32614.10	(0.10)	24(3,21) - 24(2,22)	1	A	[81037]
	32681.50	(0.10)	16(2,15) - 15(3,12)	0	E	[81037]
	32685.44	(0.10)	16(2,15) - 15(3,12)	0	A	[81037]
	32780.88	(0.10)	24(3,21) - 24(2,22)	0	E	[81037]
	32797.49	(0.10)	24(3,21) - 24(2,22)	0	A	[81037]
	32855.04	(0.10)	21(3,18) - 21(2,19)	0	A	[81037]
	32860.33	(0.10)	21(3,18) - 21(2,19)	0	E	[81037]
	32985.09	(0.10)	19(3,16) - 19(2,17)	1	A	[81037]
	32994.58	(0.10)	19(3,16) - 19(2,17)	1	E	[81037]
	33094.76	(0.10)	22(2,20) - 22(1,21)	0	E	[81037]
	33182.81	(0.10)	22(2,20) - 22(1,21)	0	A	[81037]
	33238.70	(0.10)	11(2,10) - 11(1,11)	1	E	[81037]
	33270.14	(0.10)	25(3,22) - 25(2,23)	0	E	[81037]
	33279.78	(0.10)	11(2,10) - 11(1,11)	1	A	[81037]
	33292.74	(0.10)	11(2,10) - 11(1,11)	0	E	[81037]
	33296.88	(0.10)	25(3,22) - 25(2,23)	0	A	[81037]
	33307.29	(0.10)	25(3,22) - 25(2,23)	1	E	[81037]
	33310.89	(0.10)	20(3,17) - 20(2,18)	0	A	[81037]
	33321.14	(0.10)	20(3,17) - 20(2,18)	0	E	[81037]
	33334.75	(0.10)	11(2,10) - 11(1,11)	0	A	[81037]
	33340.90	(0.10)	25(3,22) - 25(2,23)	1	A	[81037]
	33449.36	(0.10)	17(3,15) - 17(2,15)	0	A	[81037]
	33454.76	(0.10)	17(3,15) - 17(2,15)	0	E	[81037]
	33602.51	(0.10)	16(3,14) - 16(2,14)	1	E	[81037]
	33606.11	(0.10)	16(3,14) - 16(2,14)	1	A	[81037]
	33647.45	(0.10)	8(0, 8) - 7(1, 7)	0	E	[81037]
	33656.67	(0.10)	8(0, 8) - 7(1, 7)	0	A	[81037]
	33669.63	(0.10)	18(3,15) - 18(2,16)	1	A	[81037]
	33682.92	(0.10)	18(3,15) - 18(2,16)	1	E	[81037]
	33919.68	(0.10)	17(1,16) - 17(0, 7)	0	E	[81037]
	33933.79	(0.10)	19(3,16) - 19(2,17)	0	A	[81037]
	33948.27	(0.10)	19(3,16) - 19(2,17)	0	E	[81037]
	34011.37	(0.10)	17(1,16) - 17(0, 7)	0	A	[81037]
	34086.25	(0.10)	26(3,23) - 26(2,24)	0	A	[81037]
	34048.02	(0.10)	26(3,23) - 26(2,24)	0	E	[81037]
	34251.98	(0.10)	14(2,12) - 13(3,11)	1	A	[81037]
	34296.07	(0.10)	14(2,12) - 13(3,11)	1	E	[81037]
	34302.51	(0.10)	22(2,20) - 22(1,21)	1	E	[81037]
	34331.75	(0.10)	26(3,23) - 26(2,24)	1	E	[81037]
	34349.38	(0.10)	8(0, 8) - 7(1, 7)	1	E	[81037]
	34358.25	(0.10)	8(0, 8) - 7(1, 7)	1	A	[81037]
	34377.06	(0.10)	26(3,23) - 26(2,24)	1	A	[81037]
	34391.50	(0.10)	22(2,20) - 22(1,21)	1	A	[81037]
	34474.03	(0.10)	17(3,14) - 17(2,15)	1	A	[81037]
	34491.05	(0.10)	17(3,14) - 17(2,15)	1	E	[81037]
	34687.58	(0.10)	18(3,15) - 18(2,16)	0	A	[81037]

TABLE 53.3. Microwave spectrum of 2-pentene — Continued

C₅H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_-,K_-)$	$- J''(K_+,K_+)$	V_i	Sym.	Ref.
	34705.91	(0.10)	18(3,15)	- 18(2,16)	0	<i>E</i>	[81037]
	34734.33	(0.10)	12(2,11)	- 12(1,12)	0	<i>E</i>	[81037]
	34748.74	(0.10)	12(2,11)	- 12(1,12)	1	<i>E</i>	[81037]
	34779.71	(0.10)	12(2,11)	- 12(1,12)	0	<i>A</i>	[81037]
	34793.30	(0.10)	12(2,11)	- 12(1,12)	1	<i>A</i>	[81037]
	34934.18	(0.10)	16(3,14)	- 16(2,14)	0	<i>E</i>	[81037]
	34942.06	(0.10)	16(3,14)	- 16(2,14)	0	<i>A</i>	[81037]
	35034.04	(0.10)	15(3,13)	- 15(2,13)	1	<i>E</i>	[81037]
	35051.11	(0.10)	17(1,16)	- 17(0,17)	1	<i>E</i>	[81037]
	35051.94	(0.10)	15(3,13)	- 15(2,13)	1	<i>A</i>	[81037]
	35126.81	(0.10)	27(3,24)	- 27(2,25)	0	<i>E</i>	[81037]
	35137.61	(0.10)	17(1,16)	- 17(0,17)	1	<i>A</i>	[81037]
	35177.89	(0.10)	27(3,24)	- 27(2,25)	0	<i>A</i>	[81037]
	35329.15	(0.10)	2(2, 1)	- 1(1, 0)	0	<i>A</i>	[81037]
	35356.39	(0.10)	16(3,13)	- 16(2,14)	1	<i>A</i>	[81037]
	35378.03	(0.10)	16(3,13)	- 16(2,14)	1	<i>E</i>	[81037]
	35533.58	(0.10)	17(3,14)	- 17(2,15)	0	<i>A</i>	[81037]
	35556.15	(0.10)	17(3,14)	- 17(2,15)	0	<i>E</i>	[81037]
	35563.99	(0.10)	2(2, 0)	- 1(1, 1)	0	<i>A</i>	[81037]
	35673.36	(0.10)	27(3,24)	- 27(2,25)	1	<i>E</i>	[81037]
	35701.65	(0.10)	23(2,21)	- 23(1,22)	0	<i>E</i>	[81037]
	35731.59	(0.10)	27(3,24)	- 27(2,25)	1	<i>A</i>	[81037]
	35802.38	(0.10)	23(2,21)	- 23(1,22)	0	<i>A</i>	[81037]
	36015.13	(0.10)	6(1, 6)	- 5(0, 5)	0	<i>E</i>	[81037]
	36016.41	(0.10)	6(1, 6)	- 5(0, 5)	0	<i>A</i>	[81037]
	36136.76	(0.10)	6(1, 6)	- 5(0, 5)	1	<i>E</i>	[81037]
	36138.22	(0.10)	6(1, 6)	- 5(0, 5)	1	<i>A</i>	[81037]
	36170.76	(0.10)	11(1,10)	- 10(2, 9)	0	<i>E</i>	[81037]
	36181.83	(0.10)	11(1,10)	- 10(2, 9)	0	<i>A</i>	[81037]
	36274.69	(0.10)	15(3,12)	- 15(2,13)	1	<i>A</i>	[81037]
	36282.84	(0.10)	15(3,13)	- 15(2,13)	0	<i>E</i>	[81037]
	36295.16	(0.10)	13(2,12)	- 13(1,13)	0	<i>E</i>	[81037]
	36303.00	(0.10)	15(3,12)	- 15(2,13)	1	<i>E</i>	[81037]
	36307.45	(0.10)	15(3,13)	- 15(2,13)	0	<i>A</i>	[81037]
	36344.60	(0.10)	13(2,12)	- 13(1,13)	0	<i>A</i>	[81037]
	36381.93	(0.10)	13(2,12)	- 13(1,13)	1	<i>E</i>	[81037]
	36389.79	(0.10)	17(2,16)	- 16(3,13)	0	<i>A</i>	[81037]
	36404.34	(0.10)	17(2,16)	- 16(3,13)	0	<i>E</i>	[81037]
	36430.80	(0.10)	13(2,12)	- 13(1,13)	1	<i>A</i>	[81037]
	36432.42	(0.10)	16(3,13)	- 16(2,14)	0	<i>A</i>	[81037]
	36460.54	(0.10)	16(3,13)	- 16(2,14)	0	<i>E</i>	[81037]
	36514.67	(0.10)	28(3,25)	- 28(2,26)	0	<i>E</i>	[81037]
	36579.76	(0.10)	28(3,25)	- 28(2,26)	0	<i>A</i>	[81037]
	37062.00	(0.10)	18(1,17)	- 18(0,18)	0	<i>E</i>	[81037]
	37100.97	(0.10)	23(2,21)	- 23(1,22)	1	<i>E</i>	[81037]
	37161.24	(0.10)	18(1,17)	- 18(0,18)	0	<i>A</i>	[81037]
	37188.74	(0.10)	14(3,11)	- 14(2,12)	1	<i>A</i>	[81037]
	37201.47	(0.10)	23(2,21)	- 23(1,22)	1	<i>A</i>	[81037]
	37227.37	(0.10)	14(3,11)	- 14(2,12)	1	<i>E</i>	[81037]
	37335.94	(0.10)	28(3,25)	- 28(2,26)	1	<i>E</i>	[81037]
	37345.40	(0.10)	15(3,12)	- 15(2,13)	0	<i>A</i>	[81037]
	37381.78	(0.10)	15(3,12)	- 15(2,13)	0	<i>E</i>	[81037]
	37408.18	(0.10)	28(3,25)	- 28(2,26)	1	<i>A</i>	[81037]
	37488.12	(0.10)	14(3,12)	- 14(2,12)	0	<i>E</i>	[81037]
	37534.46	(0.10)	14(3,12)	- 14(2,12)	0	<i>A</i>	[81037]
	37581.38	(0.10)	11(1,10)	- 10(2, 9)	1	<i>A</i>	[81037]
	37972.40	(0.10)	14(2,13)	- 14(1,14)	0	<i>E</i>	[81037]
	38026.70	(0.10)	14(2,13)	- 14(1,14)	0	<i>A</i>	[81037]
	38062.20	(0.10)	13(3,10)	- 13(2,11)	1	<i>A</i>	[81037]
	38116.72	(0.10)	13(3,10)	- 13(2,11)	1	<i>E</i>	[81037]
	38134.77	(0.10)	14(2,13)	- 14(1,14)	1	<i>E</i>	[81037]
	38188.66	(0.10)	14(2,13)	- 14(1,14)	1	<i>A</i>	[81037]
	38214.70	(0.10)	29(3,26)	- 29(2,27)	0	<i>E</i>	[81037]
	38236.55	(0.10)	14(3,11)	- 14(2,12)	0	<i>A</i>	[81037]
	38276.94	(0.10)	18(1,17)	- 18(0,18)	1	<i>E</i>	[81037]
	38285.71	(0.10)	14(3,11)	- 14(2,12)	0	<i>E</i>	[81037]
	38294.87	(0.10)	29(3,26)	- 29(2,27)	0	<i>A</i>	[81037]

TABLE 53.3. Microwave spectrum of 2-pentene — Continued

C₅H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_-,K_-) - J''(K_+,K_+)$	V_i	Sym.	Ref.
	38369.32	(0.10)	18(1,17) - 18(0,18)	1	A	[81037]
	38414.00	(0.10)	15(2,13) - 14(3,12)	0	A	[81037]
	38442.08	(0.10)	15(2,13) - 14(3,12)	0	E	[81037]
	38535.41	(0.10)	24(2,22) - 24(1,23)	0	E	[81037]
	38648.49	(0.10)	24(2,22) - 24(1,23)	0	A	[81037]
	40286.60	(0.10)	7(1, 7) - 6(0, 6)	0	A	[81037]
	40287.08	(0.10)	7(1, 7) - 6(0, 6)	0	E	[81037]
	40444.04	(0.10)	7(1, 7) - 6(0, 6)	1	A	[81037]
	40444.16	(0.10)	7(1, 7) - 6(0, 6)	1	E	[81037]
	40594.36	(0.10)	15(2,13) - 4(3,12)	1	A	[81037]
	40613.06	(0.10)	15(2,13) - 3,12)	1	E	[81037]

Table 54.1. Molecular constants for the C₆H radical in the ²Π₁ state. [88001]

Parameter	Value
A _{eff} (GHz)	453.048(525)
B ₀ (MHz)	1391.1860(4)
D ₀ (kHz)	0.04056(5)
γ _{eff} (MHz)	-220.(2)
p (MHz)	25.36(21)
p _D (kHz)	-2.92(6)
p _H (Hz)	91.9(62)
q (MHz)	1.462(6)
q _D (kHz)	-0.015(2)
q _H (Hz)	-0.18(18)
a+(b+c)/2 (MHz)	3.205(71) ^a

^aFrom reference [87006].

TABLE 54.2. Microwave spectrum of C₆H radicalC₆H

Isotopic Species	Frequency (MHz)	Unc. (MHz)	$J' - J''$	P	$F' - F''$	Vib. State	Ref.
CCCCCCH $^2\Pi_{3/2}$	20792.872	(0.020)	15/2 - 13/2	<i>f</i>	8 - 7	$\nu = 0$	[87007]
	20792.944	(0.020)	15/2 - 13/2	<i>f</i>	7 - 6	$\nu = 0$	[87007]
	20794.441	(0.020)	15/2 - 13/2	<i>e</i>	8 - 7	$\nu = 0$	[87007]
	20794.511	(0.020)	15/2 - 13/2	<i>e</i>	7 - 6	$\nu = 0$	[87007]
	23565.160	(0.020)	17/2 - 15/2	<i>f</i>	9 - 8	$\nu = 0$	[86022]
	23565.226	(0.020)	17/2 - 15/2	<i>f</i>	8 - 7	$\nu = 0$	[86022]
	23567.169	(0.020)	17/2 - 15/2	<i>e</i>	9 - 8	$\nu = 0$	[86022]
	23567.238	(0.020)	17/2 - 15/2	<i>e</i>	8 - 7	$\nu = 0$	[86022]
	40198.356	(0.030)	29/2 - 27/2	<i>f</i>		$\nu = 0$	[86022]
	40204.150	(0.030)	29/2 - 27/2	<i>e</i>		$\nu = 0$	[86022]
	42970.453	(0.030)	31/2 - 29/2	<i>f</i>		$\nu = 0$	[86022]
	42977.115	(0.020)	31/2 - 29/2	<i>e</i>		$\nu = 0$	[86022]
	73460.	(1.0)	53/2 - 51/2	<i>f</i>		$\nu = 0$	[87007]
	73480.5	(1.0)	53/2 - 51/2	<i>e</i>		$\nu = 0$	[87007]
	81778.1	(0.3)	59/2 - 57/2	<i>f</i>		$\nu = 0$	[87007]
	81801.1	(0.3)	59/2 - 57/2	<i>e</i>		$\nu = 0$	[87007]
	84549.9	(0.4)	61/2 - 59/2	<i>f</i>		$\nu = 0$	[87007]
	84574.5	(0.5)	61/2 - 59/2	<i>e</i>		$\nu = 0$	[87007]
	87348.3	(0.5)	63/2 - 61/2	<i>e</i>		$\nu = 0$	[87007]
	90093.0	(0.4)	65/2 - 63/2	<i>f</i>		$\nu = 0$	[87007]
	90121.4	(0.5)	65/2 - 63/2	<i>e</i>		$\nu = 0$	[87007]
	92865.2	(0.3)	67/2 - 65/2	<i>f</i>		$\nu = 0$	[87007]
	92894.9	(0.3)	67/2 - 65/2	<i>e</i>		$\nu = 0$	[87007]
	95636.6	(0.3)	69/2 - 67/2	<i>f</i>		$\nu = 0$	[87007]
	95668.3	(0.6)	69/2 - 67/2	<i>e</i>		$\nu = 0$	[87007]
	98408.9	(0.4)	71/2 - 69/2	<i>f</i>		$\nu = 0$	[87007]
	98441.7	(0.5)	71/2 - 69/2	<i>e</i>		$\nu = 0$	[87007]
	101180.3	(0.3)	72/2 - 71/2	<i>f</i>		$\nu = 0$	[87009]
	101251.9	(1.5)	72/2 - 71/2	<i>e</i>		$\nu = 0$	[87009]
	103951.9	(0.4)	75/2 - 73/2	<i>f</i>		$\nu = 0$	[87009]
	103989.0	(0.4)	75/2 - 73/2	<i>e</i>		$\nu = 0$	[87009]
	106762.7	(0.3)	75/2 - 75/2	<i>e</i>		$\nu = 0$	[87009]
	115038.4	(0.7)	83/2 - 81/2	<i>f</i>		$\nu = 0$	[87009]
	115084.0	(0.7)	83/2 - 81/2	<i>e</i>		$\nu = 0$	[87009]
CCCCCCH $^2\Pi_{1/2}$	43261.60	(0.30)	31/2 - 29/2	<i>f</i>		$\nu = 0$	[87006]
	43294.60	(0.30)	31/2 - 29/2	<i>e</i>		$\nu = 0$	[87006]
	73967.00	(0.30)	53/2 - 51/2	<i>f</i>		$\nu = 0$	[86024]
	74008.00	(0.30)	53/2 - 51/2	<i>e</i>		$\nu = 0$	[86024]
	82384.5	(0.5)	59/2 - 57/2	<i>e</i>		$\nu = 0$	[87009]
	85131.1	(0.4)	61/2 - 59/2	<i>f</i>		$\nu = 0$	[87009]
	85176.0	(0.4)	61/2 - 59/2	<i>e</i>		$\nu = 0$	[87009]
	87921.7	(0.3)	63/2 - 61/2	<i>f</i>		$\nu = 0$	[87009]
	87967.7	(0.3)	63/2 - 61/2	<i>e</i>		$\nu = 0$	[87009]
	90712.2	(0.3)	65/2 - 63/2	<i>f</i>		$\nu = 0$	[87009]
	90759.3	(0.3)	65/2 - 63/2	<i>e</i>		$\nu = 0$	[87009]
	93502.2	(1.0)	67/2 - 65/2	<i>f</i>		$\nu = 0$	[87009]
	93550.9	(0.5)	67/2 - 65/2	<i>e</i>		$\nu = 0$	[87009]
	96293.3	(0.3)	69/2 - 67/2	<i>f</i>		$\nu = 0$	[87006]
	96342.5	(0.3)	69/2 - 67/2	<i>e</i>		$\nu = 0$	[87006]
	99083.9	(0.3)	71/2 - 69/2	<i>f</i>		$\nu = 0$	[87006]
	99134.1	(0.3)	71/2 - 69/2	<i>e</i>		$\nu = 0$	[87006]
	101873.6	(1.0)	73/2 - 71/2	<i>f</i>		$\nu = 0$	[87009]
	101925.2	(0.7)	73/2 - 71/2	<i>e</i>		$\nu = 0$	[87009]
	107453.2	(0.3)	77/2 - 75/2	<i>f</i>		$\nu = 0$	[87009]
	107507.9	(0.4)	77/2 - 75/2	<i>e</i>		$\nu = 0$	[87009]
	110229.8	(1.0)	79/2 - 77/2	<i>e</i>		$\nu = 0$	[87009]
	110243.4	(1.0)	79/2 - 77/2	<i>f</i>		$\nu = 0$	[87009]

Table 55.1. Molecular constants for o-benzyne.

Parameter	Value (present)	Parameter	Value [86005]
A'' (MHz)	6989.713(16)	A (MHz)	6989.665(8)
B'' (MHz)	5706.795(14)	B (MHz)	5706.759(7)
C'' (MHz)	3140.368(6)	C (MHz)	3140.384(4)
τ_1 (kHz)	-8.76(406)	D _{JK} (kHz)	1.55(1)
τ_2 (kHz)	-2.00(136)	d ₂ (kHz)	-0.241(3)
τ_3^a (kHz)	92.6(168)		
τ_{aaaa} (kHz)	-9.29(102)		
τ_{bbbb} (kHz)	-4.55(120)		

^aValue determined from planarity conditions.

TABLE 55.2. Microwave spectrum of benzyne

C₆H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
CHCCCHCHCH	27590.480	(0.060)	15(9, 6) - 15(8, 7)	[86005]
	27717.040	(0.060)	12(9, 3) - 12(8, 4)	[86005]
	28230.170	(0.060)	4(0, 4) - 3(1, 3)	[86005]
	28440.700	(0.060)	14(10, 4) - 14(9, 5)	[86005]
	29066.150	(0.060)	16(11, 5) - 16(10, 6)	[86005]
	29292.500	(0.060)	19(12, 7) - 19(11, 8)	[86005]
	29868.000	(0.060)	18(12, 6) - 18(11, 7)	[86005]
	30109.860	(0.060)	18(11, 7) - 18(10, 8)	[86005]
	30462.930	(0.060)	10(5, 5) - 10(4, 6)	[86005]
	30576.710	(0.060)	14(8, 6) - 14(7, 7)	[86005]
	31110.020	(0.060)	20(13, 7) - 20(12, 8)	[86005]
	31801.340	(0.060)	11(8, 4) - 11(7, 5)	[86005]
	40828.180	(0.060)	6(0, 6) - 5(1, 5)	[86005]
	40830.000	(0.060)	6(1, 6) - 5(0, 5)	[86005]

Table 56.1. Molecular constants for 3,4-dimethylenecyclobutene, $\text{CH}=\text{CHC}(\text{CH}_2)\text{C}(\text{=CH}_2)$.

Parameter	Value	Parameter ^a	Value ^a
A'' (MHz)	5569.8998(17)	A (MHz)	5569.896(1)
B'' (MHz)	4161.7995(14)	B (MHz)	4161.804(1)
C'' (MHz)	2413.5376(9)	C (MHz)	2413.545(1)
τ_1 (kHz)	4.28(43)	D _J (kHz)	1.49(1)
τ_2 (kHz)	0.485(129)	D _{JK} (kHz)	-5.51(5)
τ_3^b (kHz)	39.8(32)	D _K (kHz)	7.52(8)
τ_{aaaa} (kHz)	-14.1(4)	d ₁ (kHz)	-0.672(4)
τ_{bbbb} (kHz)	-11.20(14)		
τ_{cccc} (kHz)	0 ^c		
<u>Electric Dipole Moment [83033]</u>			
μ_b (D)	0.6157(20)		

^aThis set of parameters and values are from reference [83033] and are given so comparisons can be made with the ¹³C and D species in Tables 54.2 and 54.3.

^bValue fixed by setting R₆ = 0.

^cFixed at zero.

Table 56.2. Molecular constants for the ¹³C substituted species of 3,4-dimethylenecyclobutene. [83033]

Parameter	1- ¹³ C	3- ¹³ C	5- ¹³ C
A (MHz)	5467.639(17)	5568.505(8)	5505.316(15)
B (MHz)	4244.140(11)	4241.941(9)	4156.629(17)
C (MHz)	2388.553(3)	2406.898(2)	2367.548(5)
D _J (kHz)	1.35(19)	1.43(9)	1.02(24)
D _{JK} (kHz)	-4.53(77)	-5.49(45)	-3.89(77)
D _K (kHz)	6.20(164)	7.97(73)	7.92(12)
d ₁ (kHz)	-0.619(108)	-0.708(55)	-0.445(132)

Table 56.3. Molecular constants for the deuterated isotopes of 3,4-dimethylenecyclobutene. [83033]

Parameter	1,2-d ₂	E-5-d ₁	Z-5-d ₁
A (MHz)	5084.403(3)	5538.362(2)	5323.761(2)
B (MHz)	4118.900(4)	4002.134(2)	4175.687(5)
C (MHz)	2274.799(2)	2322.471(1)	2339.355(1)
D _J (kHz)	1.38(12)	1.26(3)	1.55(5)
D _{JK} (kHz)	-4.87(12)	-4.26(13)	-5.42(26)
D _K (kHz)	6.36(16)	6.57(22)	6.95(39)
d ₁ (kHz)	-0.600(66)	-0.579(11)	-0.691(28)

TABLE 56.4. Microwave spectrum of 3,4-dimethylenecyclobutene

C₆H₆

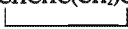
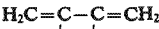

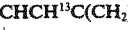
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.	
$\text{CHCHC}(\text{CH}_2)\text{C}(\text{CH}_2)$ 	19123.19	(0.05)	2(2, 1) - 1(1, 0)	[83033]	
	19601.66	(0.05)	7(5, 3) - 7(4, 4)	[83033]	
	21467.28	(0.05)	7(4, 4) - 7(3, 5)	[83033]	
	21656.01	(0.05)	4(0, 4) - 3(1, 3)	[83033]	
	$\text{H}_2\text{C}=\text{C}-\text{C}=\text{CH}_2$  $\text{HC}=\text{CH}$	21806.15	(0.05)	4(1, 4) - 3(0, 3)	[83033]
		22000.57	(0.05)	2(2, 0) - 1(1, 1)	[83033]
	22885.04	(0.05)	4(2, 2) - 3(3, 1)	[83033]	
	23950.30	(0.05)	3(2, 2) - 2(1, 1)	[83033]	
	25047.20	(0.05)	4(1, 3) - 3(2, 2)	[83033]	
	26539.20	(0.05)	5(0, 5) - 4(1, 4)	[83033]	
	26569.96	(0.05)	5(1, 5) - 4(0, 4)	[83033]	
	27953.26	(0.05)	4(2, 3) - 3(1, 2)	[83033]	
	27953.26	(0.05)	4(2, 3) - 3(1, 2)	[83033]	
	30692.98	(0.05)	3(3, 1) - 2(2, 0)	[83033]	
	30934.89	(0.05)	5(1, 4) - 4(2, 3)	[83033]	
	31377.14	(0.05)	6(0, 6) - 5(1, 5)	[83033]	
	31382.85	(0.05)	6(1, 6) - 5(0, 5)	[83033]	
	31867.24	(0.05)	5(2, 3) - 4(3, 2)	[83033]	
	31943.06	(0.05)	5(2, 4) - 4(1, 3)	[83033]	
	32151.72	(0.05)	3(3, 0) - 2(2, 1)	[83033]	
	33466.81	(0.05)	3(2, 1) - 2(1, 2)	[83033]	
	35748.51	(0.05)	4(3, 2) - 3(2, 1)	[83033]	
	36110.34	(0.05)	6(1, 5) - 5(2, 4)	[83033]	
	36380.24	(0.05)	6(2, 5) - 5(1, 4)	[83033]	
	36689.49	(0.05)	6(3, 3) - 5(4, 2)	[83033]	
	39365.39	(0.05)	6(2, 4) - 5(3, 3)	[83033]	
	39620.79	(0.05)	5(3, 3) - 4(2, 2)	[83033]	
	$^{13}\text{CHCHC}(\text{CH}_2)\text{C}(\text{CH}_2)$ 	18791.45	(0.05)	2(2, 1) - 1(1, 0)	[83033]
21196.74		(0.05)	7(4, 4) - 7(3, 5)	[83033]	
21442.56		(0.05)	4(0, 4) - 3(1, 3)	[83033]	
21568.01		(0.05)	4(1, 4) - 3(0, 3)	[83033]	
23207.19		(0.05)	4(2, 2) - 3(3, 1)	[83033]	
23568.54		(0.05)	3(2, 2) - 2(1, 1)	[83033]	
24956.44		(0.05)	4(1, 3) - 3(2, 2)	[83033]	
26267.03		(0.05)	5(0, 5) - 4(1, 4)	[83033]	
26291.33		(0.05)	5(1, 5) - 4(0, 4)	[83033]	
27535.36		(0.05)	4(2, 3) - 3(1, 2)	[83033]	
30139.98		(0.05)	3(3, 1) - 2(2, 0)	[83033]	
30685.90		(0.05)	5(1, 4) - 4(2, 3)	[83033]	
31052.67		(0.05)	6(0, 6) - 5(1, 5)	[83033]	
31056.94		(0.05)	6(1, 6) - 5(0, 5)	[83033]	
31533.76		(0.05)	5(2, 4) - 4(1, 3)	[83033]	
31673.97		(0.05)	3(3, 0) - 2(2, 1)	[83033]	
31991.32		(0.05)	5(2, 3) - 4(3, 2)	[83033]	
33208.71		(0.05)	3(2, 1) - 2(1, 2)	[83033]	
35123.19		(0.05)	4(3, 2) - 3(2, 1)	[83033]	
35758.58		(0.05)	6(1, 5) - 5(2, 4)	[83033]	
35973.10		(0.05)	6(2, 5) - 5(1, 4)	[83033]	
37165.39		(0.05)	6(3, 3) - 5(4, 2)	[83033]	
38937.17		(0.05)	5(3, 3) - 4(2, 2)	[83033]	
$\text{CHCH}^{13}\text{C}(\text{CH}_2)\text{C}(\text{CH}_2)$ 		19112.46	(0.05)	2(2, 1) - 1(1, 0)	[83033]
		21425.95	(0.05)	7(4, 4) - 7(3, 5)	[83033]
		21592.78	(0.05)	4(0, 4) - 3(1, 3)	[83033]
		21750.22	(0.05)	4(1, 4) - 3(0, 3)	[83033]
		21958.80	(0.05)	2(2, 0) - 1(1, 1)	[83033]
	22648.10	(0.05)	4(2, 2) - 3(3, 1)	[83033]	
	23926.20	(0.05)	3(2, 2) - 2(1, 1)	[83033]	
	24923.91	(0.05)	4(1, 3) - 3(2, 2)	[83033]	
	26465.27	(0.05)	5(0, 5) - 4(1, 4)	[83033]	
	26498.05	(0.05)	5(1, 5) - 4(0, 4)	[83033]	
	27916.93	(0.05)	4(2, 3) - 3(1, 2)	[83033]	
	30681.77	(0.05)	3(3, 1) - 2(2, 0)	[83033]	
	30825.95	(0.05)	5(1, 4) - 4(2, 3)	[83033]	
	31290.64	(0.05)	6(0, 6) - 5(1, 5)	[83033]	
	31296.83	(0.05)	6(1, 6) - 5(0, 5)	[83033]	
	31635.00	(0.05)	5(2, 3) - 4(3, 2)	[83033]	
	31880.88	(0.05)	5(2, 4) - 4(1, 3)	[83033]	
	32109.73	(0.05)	3(3, 0) - 2(2, 1)	[83033]	

TABLE 56.4. Microwave spectrum of 3,4-dimethylenecyclobutene — Continued

C₆H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
	33348.54	(0.05)	3(2, 1) - 2(1, 2)	[83033]
	35729.63	(0.05)	4(3, 2) - 3(2, 1)	[83033]
	36003.25	(0.05)	6(1, 5) - 5(2, 4)	[83033]
	36290.49	(0.05)	6(2, 5) - 5(1, 4)	[83033]
	36319.75	(0.05)	6(3, 3) - 5(4, 2)	[83033]
	39172.16	(0.05)	6(2, 4) - 5(3, 3)	[83033]
	39597.35	(0.05)	5(3, 3) - 4(2, 2)	[83033]
CHCHC(¹³ CH ₂)C(CH ₂)	18883.41	(0.05)	2(2, 1) - 1(1, 0)	[83033]
	21115.75	(0.05)	7(4, 4) - 7(3, 5)	[83033]
	21638.60	(0.05)	2(2, 0) - 1(1, 1)	[83033]
	21232.17	(0.05)	4(0, 4) - 3(1, 3)	[83033]
	21403.20	(0.05)	4(1, 4) - 3(0, 3)	[83033]
	23618.53	(0.05)	3(2, 2) - 2(1, 1)	[83033]
	24406.11	(0.05)	4(1, 3) - 3(2, 2)	[83033]
	26030.62	(0.05)	5(0, 5) - 4(1, 4)	[83033]
	26067.39	(0.05)	5(1, 5) - 4(0, 4)	[83033]
	27542.01	(0.05)	4(2, 3) - 3(1, 2)	[83033]
	30272.50	(0.05)	5(1, 4) - 4(2, 3)	[83033]
	30326.22	(0.05)	3(3, 1) - 2(2, 0)	[83033]
	30778.70	(0.05)	6(0, 6) - 5(1, 5)	[83033]
	30785.88	(0.05)	6(1, 6) - 5(0, 5)	[83033]
	30827.13	(0.05)	5(2, 3) - 4(3, 2)	[83033]
	31412.68	(0.05)	5(2, 4) - 4(1, 3)	[83033]
	31679.43	(0.05)	3(3, 0) - 2(2, 1)	[83033]
	32754.01	(0.05)	3(2, 1) - 2(1, 2)	[83033]
	35303.77	(.05)	4(3, 2) - 3(2, 1)	[83033]
	35398.23	(0.05)	6(1, 5) - 5(2, 4)	[83033]
	35719.13	(0.05)	6(2, 5) - 5(1, 4)	[83033]
CDCDC(CH ₂)C(CH ₂)	39120.94	(0.05)	5(3, 3) - 4(2, 2)	[83033]
	8428.78	(0.05)	2(2, 1) - 2(1, 2)	[83033]
	8592.33	(0.05)	6(4, 2) - 6(3, 3)	[83033]
	8658.82	(0.05)	5(3, 2) - 5(2, 3)	[83033]
	9513.27	(0.05)	4(2, 2) - 4(1, 3)	[83033]
	9516.25	(0.05)	4(4, 0) - 4(3, 1)	[83033]
	9735.79	(0.05)	7(5, 2) - 7(4, 3)	[83033]
	10038.23	(0.05)	3(3, 1) - 3(2, 2)	[83033]
	10537.25	(0.05)	3(1, 2) - 3(0, 3)	[83033]
	10651.91	(0.05)	2(0, 2) - 1(1, 1)	[83033]
	10982.25	(0.05)	6(5, 1) - 6(4, 2)	[83033]
	11225.64	(0.05)	8(5, 3) - 8(4, 4)	[83033]
	11614.13	(0.05)	9(6, 3) - 9(5, 4)	[83033]
	11795.53	(0.05)	3(2, 2) - 3(1, 3)	[83033]
	11908.81	(0.05)	2(1, 2) - 1(0, 1)	[83033]
	12027.61	(0.05)	7(4, 3) - 7(3, 4)	[83033]
	12244.86	(0.05)	8(6, 2) - 8(5, 3)	[83033]
	15756.26	(0.05)	3(0, 3) - 2(1, 2)	[83033]
	16105.67	(0.05)	3(1, 3) - 2(0, 2)	[83033]
	17864.73	(0.05)	3(1, 2) - 2(2, 1)	[83033]
	20445.17	(0.05)	4(0, 4) - 3(1, 3)	[83033]
	20512.77	(0.05)	4(1, 4) - 3(0, 3)	[83033]
<i>c</i> -CHCHC(CHD)C(CH ₂)	18931.37	(0.05)	6(2, 4) - 6(1, 5)	[83033]
	18937.51	(0.05)	2(2, 1) - 1(1, 0)	[83033]
	19140.36	(0.05)	5(5, 0) - 5(4, 1)	[83033]
	20482.87	(0.05)	8(6, 2) - 8(5, 3)	[83033]
	20485.51	(0.05)	7(5, 3) - 7(4, 4)	[83033]
	20782.96	(0.05)	4(0, 4) - 3(1, 3)	[83033]
	20989.25	(0.05)	7(4, 4) - 7(3, 5)	[83033]
	21044.86	(0.05)	4(1, 4) - 3(0, 3)	[83033]
	21436.95	(0.05)	2(2, 0) - 1(1, 1)	[83033]
	23353.94	(0.05)	4(1, 3) - 3(2, 2)	[83033]
	23582.46	(0.05)	3(2, 2) - 2(1, 1)	[83033]
	24663.64	(0.05)	8(4, 5) - 8(3, 6)	[83033]
	24905.33	(0.05)	9(5, 5) - 9(4, 6)	[83033]
	25521.99	(0.05)	5(0, 5) - 4(1, 4)	[83033]
	25586.98	(0.05)	5(1, 5) - 4(0, 4)	[83033]
	27431.21	(0.05)	4(2, 3) - 3(1, 2)	[83033]
	28746.71	(0.05)	5(2, 3) - 4(3, 2)	[83033]

TABLE 56.4. Microwave spectrum of 3,4-dimethylenecyclobutene -- Continued

C₆H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
z-CHCHC(CHD)C(CH ₂) ┌──────────┘	29406.92	(0.05)	5(1, 4) - 4(2, 3)	[83033]
	30189.67	(0.05)	6(0, 6) - 5(1, 5)	[83033]
	30204.32	(0.05)	6(1, 6) - 5(0, 5)	[83033]
	30466.25	(0.05)	3(3, 1) - 2(2, 0)	[83033]
	31107.59	(0.05)	5(2, 4) - 4(1, 3)	[83033]
	31574.11	(0.05)	3(3, 0) - 2(2, 1)	[83033]
	31860.24	(0.05)	6(3, 3) - 5(4, 2)	[83033]
	31925.37	(0.05)	3(2, 1) - 2(1, 2)	[83033]
	34617.19	(0.05)	6(1, 5) - 5(2, 4)	[83033]
	34839.15	(0.05)	7(0, 7) - 6(1, 6)	[83033]
	34842.24	(0.05)	7(1, 7) - 6(0, 6)	[83033]
	35173.39	(0.05)	6(2, 5) - 5(1, 4)	[83033]
	35409.88	(0.05)	4(3, 2) - 3(2, 1)	[83033]
	36637.59	(0.05)	6(2, 4) - 5(3, 3)	[83033]
	39223.94	(0.05)	5(3, 3) - 4(2, 2)	[83033]
	18310.60	(0.05)	2(2, 1) - 1(1, 0)	[83033]
	18392.67	(0.05)	7(5, 3) - 7(4, 4)	[83033]
	20107.54	(0.05)	6(2, 4) - 6(1, 5)	[83033]
	20734.24	(0.05)	7(4, 4) - 7(3, 5)	[83033]
	21007.85	(0.05)	4(0, 4) - 3(1, 3)	[83033]
	21115.75	(0.05)	4(1, 4) - 3(0, 3)	[83033]
	21229.21	(0.05)	2(2, 0) - 1(1, 1)	[83033]
	22989.33	(0.05)	3(2, 2) - 2(1, 1)	[83033]
	24555.35	(0.05)	4(1, 3) - 3(2, 2)	[83033]
	25727.47	(0.05)	5(0, 5) - 4(1, 4)	[83033]
	25747.57	(0.05)	5(1, 5) - 4(0, 4)	[83033]
	26879.65	(0.05)	4(2, 3) - 3(1, 2)	[83033]
	29353.44	(0.05)	3(3, 1) - 2(2, 0)	[83033]
	30099.30	(0.05)	5(1, 4) - 4(2, 3)	[83033]
	30413.22	(0.05)	6(0, 6) - 5(1, 5)	[83033]
	30416.62	(0.05)	6(1, 6) - 5(0, 5)	[83033]
	30832.66	(0.05)	5(2, 4) - 4(1, 3)	[83033]
	30923.91	(0.05)	3(3, 0) - 2(2, 1)	[83033]
	31641.75	(0.05)	5(2, 3) - 4(3, 2)	[83033]
	32591.17	(0.05)	3(2, 1) - 2(1, 2)	[83033]
	34220.22	(0.05)	4(3, 2) - 3(2, 1)	[83033]
	35035.26	(0.05)	6(1, 5) - 5(2, 4)	[83033]
	35092.63	(0.05)	7(0, 7) - 6(1, 6)	[83033]
35093.16	(0.05)	7(1, 7) - 6(0, 6)	[83033]	
35212.95	(0.05)	6(2, 5) - 5(1, 4)	[83033]	
36993.75	(0.05)	6(3, 3) - 5(4, 2)	[83033]	
37944.21	(0.05)	5(3, 3) - 4(2, 2)	[83033]	
38572.85	(0.05)	6(2, 4) - 5(3, 3)	[83033]	

Table 57.1. Molecular constants of tricyclo[3.1.0.0^{2,6}]hex-3-ene (benzvalene).

Species	A (MHz)	B (MHz)	C (MHz)	Reference
Normal	7389.2330(73)	5275.9189(41)	3889.7787(32)	[present]
1- ¹³ C	7334.510(47)	5192.586(4)	3859.480(3)	[73076]
2- ¹³ C	7267.656(92)	5273.698(7)	3854.647(6)	[73076]
3- ¹³ C	7344.398(162)	5191.750(11)	3831.499(10)	[73076]
1-d ₁	7175.631(4)	4997.498(3)	3793.592(3)	[73076]
2-d ₁	6948.922(7)	5256.549(3)	3754.365(2)	[73076]
3-d ₁	7226.229(7)	5035.768(3)	3714.995(3)	[73076]
<u>Dipole Moment</u> [72065]				
μ_a (D)	0.883(10)			

TABLE 57.2. Microwave spectrum of tricyclo[3.1.0.0](2,6)hex-3-ene

C₆H₆



Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.	
	9165.690	(0.050)	1(0, 1) - 0(0, 0)	[72065]	
	16945.270	(0.050)	2(1, 2) - 1(1, 1)	[72065]	
	17839.510	(0.050)	2(0, 2) - 1(0, 1)	[72065]	
	18749.556	(0.050)	5(3, 3) - 5(1, 4)	[72067]	
	19714.860	(0.050)	5(2, 4) - 5(0, 5)	[72065]	
	19717.620	(0.050)	2(1, 1) - 1(1, 0)	[72065]	
	20646.480	(0.050)	6(3, 4) - 6(1, 5)	[72065]	
	25149.810	(0.050)	3(1, 3) - 2(1, 2)	[72065]	
	25834.940	(0.050)	3(0, 3) - 2(0, 2)	[72065]	
	27497.092	(0.050)	3(2, 2) - 2(2, 1)	[72067]	
	29159.212	(0.050)	3(2, 1) - 2(2, 0)	[72067]	
	29190.560	(0.050)	3(1, 2) - 2(1, 1)	[72065]	
	33162.320	(0.050)	4(1, 4) - 3(1, 3)	[72065]	
	33503.398	(0.050)	4(0, 4) - 3(0, 3)	[72067]	
	36268.079	(0.050)	4(2, 3) - 3(2, 2)	[72067]	
	¹³ CHCHCHCHCHCH	16771.04	(0.05)	2(1, 2) - 1(1, 1)	[73076]
		17648.07	(0.05)	2(0, 2) - 1(0, 1)	[73076]
		19437.27	(0.05)	2(1, 1) - 1(1, 0)	[73076]
		25594.85	(0.05)	3(0, 3) - 2(0, 2)	[73076]
		27156.21	(0.05)	3(2, 2) - 2(2, 1)	[73076]
28712.56		(0.05)	3(2, 1) - 2(2, 0)	[73076]	
28801.77		(0.05)	3(1, 2) - 2(1, 1)	[73076]	
32860.48		(0.05)	4(1, 4) - 3(1, 3)	[73076]	
33218.38		(0.05)	4(0, 4) - 3(0, 3)	[73076]	
35843.07		(0.05)	4(2, 3) - 3(2, 2)	[73076]	
CH ¹³ CHCHCHCHCH	9128.34	(0.05)	1(0, 1) - 0(0, 0)	[73076]	
	16837.64	(0.05)	2(1, 2) - 1(1, 1)	[73076]	
	17724.26	(0.05)	2(0, 2) - 1(0, 1)	[73076]	
	19675.74	(0.05)	2(1, 1) - 1(1, 0)	[73076]	
	24967.95	(0.05)	3(1, 3) - 2(1, 2)	[73076]	
	25614.64	(0.05)	3(0, 3) - 2(0, 2)	[73076]	
CHCH ¹³ CHCHCHCH	29089.26	(0.05)	3(1, 2) - 2(1, 1)	[73076]	
	16686.31	(0.05)	2(1, 2) - 1(1, 1)	[73076]	
	19406.75	(0.05)	2(1, 1) - 1(1, 0)	[73076]	
	24772.47	(0.05)	3(1, 3) - 2(1, 2)	[73076]	
	25469.15	(0.05)	3(0, 3) - 2(0, 2)	[73076]	
	27069.75	(0.05)	3(2, 2) - 2(2, 1)	[73076]	
	28744.03	(0.05)	3(1, 2) - 2(1, 1)	[73076]	
	32671.53	(0.05)	4(1, 4) - 3(1, 3)	[73076]	
	33027.60	(0.05)	4(0, 4) - 3(0, 3)	[73076]	
	35716.11	(0.05)	4(2, 3) - 3(2, 2)	[73076]	
CDCHCHCHCHCH	36793.90	(0.05)	4(3, 2) - 3(3, 1)	[73076]	
	8791.10	(0.05)	1(0, 1) - 0(0, 0)	[73076]	
	16378.29	(0.05)	2(1, 2) - 1(1, 1)	[73076]	
	17204.03	(0.05)	2(0, 2) - 1(0, 1)	[73076]	
	18786.14	(0.05)	2(1, 1) - 1(1, 0)	[73076]	
	24358.88	(0.05)	3(1, 3) - 2(1, 2)	[73076]	
	25055.09	(0.05)	3(0, 3) - 2(0, 2)	[73076]	
	26373.27	(0.05)	3(2, 2) - 2(2, 1)	[73076]	
	27691.42	(0.05)	3(2, 1) - 2(2, 0)	[73076]	
	27891.80	(0.05)	3(1, 2) - 2(1, 1)	[73076]	
CHCDCHCHCHCH	18355.81	(0.05)	5(3, 3) - 5(1, 4)	[73076]	
	18130.33	(0.05)	5(2, 4) - 5(0, 5)	[73076]	
	19606.96	(0.05)	6(3, 4) - 6(1, 5)	[73076]	
	16519.65	(0.05)	2(1, 2) - 1(1, 1)	[73076]	
	24432.66	(0.05)	3(1, 3) - 2(1, 2)	[73076]	
	24971.12	(0.05)	3(0, 3) - 2(0, 2)	[73076]	
	27032.73	(0.05)	3(2, 2) - 2(2, 1)	[73076]	
	29094.40	(0.05)	3(2, 1) - 2(2, 0)	[73076]	
	28743.05	(0.05)	3(1, 2) - 2(1, 1)	[73076]	
	32343.35	(0.05)	4(0, 4) - 3(0, 3)	[73076]	
CHCHCDCHCHCH	36952.09	(0.05)	4(3, 2) - 3(3, 1)	[73076]	
	17049.68	(0.05)	5(3, 3) - 5(1, 4)	[73076]	
	19517.05	(0.05)	5(2, 4) - 5(0, 5)	[73076]	
	19776.49	(0.05)	6(3, 4) - 6(1, 5)	[73076]	
	16180.80	(0.05)	2(1, 2) - 1(1, 1)	[73076]	
	17059.76	(0.05)	2(0, 2) - 1(0, 1)	[73076]	

TABLE 57.2. Microwave spectrum of tricyclo[3.1.0.0](2,6)hex-3-ene — Continued

C₆H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
	18822.36	(0.05)	2(1, 1) - 1(1, 0)	[73076]
	24028.96	(0.05)	3(1, 3) - 2(1, 2)	[73076]
	24735.81	(0.05)	3(0, 3) - 2(0, 2)	[73076]
	26252.29	(0.05)	3(2, 2) - 2(2, 1)	[73076]
	27768.80	(0.05)	3(2, 1) - 2(2, 0)	[73076]
	31697.35	(0.05)	4(1, 4) - 3(1, 3)	[73076]
	34649.75	(0.05)	4(2, 3) - 3(2, 2)	[73076]
	35667.14	(0.05)	4(3, 2) - 3(3, 1)	[73076]
	36209.85	(0.05)	4(3, 1) - 3(3, 0)	[73076]
	18914.76	(0.05)	5(3, 3) - 5(1, 4)	[73076]
	19330.16	(0.05)	5(2, 4) - 5(0, 5)	[73076]
	20516.47	(0.05)	6(3, 4) - 6(1, 5)	[73076]

Table 58.1. Molecular constants of 1-methylene-2,4-cyclopentadiene (fulvene).

Species	A (MHz)	B (MHz)	C (MHz)	Reference
Normal	8186.1340(89)	3802.7320(24)	2596.4362(18)	[present]
1- ¹³ C	8186.134 ^a	3786.028(15)	2588.678(15)	[72066]
2- ¹³ C	8007.593(135)	3802.505(20)	2578.126(12)	[72066]
3- ¹³ C	8117.033(178)	3748.340(23)	2664.138(14)	[72066]
6- ¹³ C	8186.134 ^a	3679.712(18)	2538.471(15)	[72066]
2-d ₁	7595.060(11)	3801.038(7)	2533.132(5)	[72066]
3-d ₁	7968.038(13)	3657.337(10)	2506.679(5)	[72066]
2,3-d ₂	7410.340(10)	3656.517(5)	2448.327(4)	[72066]
6-d ₁	8084.044(33)	3607.605(10)	2494.354(10)	[73077]
<u>Dipole Moment</u> [72066]				
μ_a (D)	0.4236(13)			

^aSet equal to A for the normal species.

TABLE 58.2. Microwave spectrum of 1-methylene-2,4-cyclopentadiene

C₆H₆

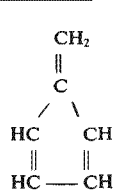
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$	$- J''(K_{-1}, K_{+1})$	Ref.	
$\text{C}(\text{CH}_2)\text{CHCHCHCH}$ 	6399.18	(0.04)	1(0, 1)	- 0(0, 0)	[72066]	
	11592.09	(0.04)	2(1, 2)	- 1(1, 1)	[72066]	
	12581.87	(0.04)	2(0, 2)	- 1(0, 1)	[72066]	
	14004.66	(0.04)	2(1, 1)	- 1(1, 0)	[72066]	
	17262.99	(0.04)	3(1, 3)	- 2(1, 2)	[72066]	
	17439.78	(0.04)	5(1, 4)	- 5(1, 5)	[72066]	
	18373.98	(0.04)	3(0, 3)	- 2(0, 2)	[72066]	
	19197.59	(0.04)	3(2, 2)	- 2(2, 1)	[72066]	
	20021.04	(0.04)	3(2, 1)	- 2(2, 0)	[72066]	
	20857.14	(0.04)	3(1, 2)	- 2(1, 1)	[72066]	
	22660.26	(0.04)	4(2, 3)	- 4(0, 4)	[72066]	
	22815.37	(0.04)	4(1, 4)	- 3(1, 3)	[72066]	
	23752.97	(0.04)	4(0, 4)	- 3(0, 3)	[72066]	
	25292.26	(0.04)	5(2, 4)	- 5(0, 5)	[72066]	
	25426.89	(0.04)	4(2, 3)	- 3(2, 2)	[72066]	
	25965.32	(0.04)	4(3, 2)	- 3(3, 1)	[72066]	
	28884.00	(0.04)	5(0, 5)	- 4(0, 4)	[72066]	
	$^{13}\text{C}(\text{CH}_2)\text{CHCHCHCH}$	11552.05	(0.04)	2(1, 2)	- 1(1, 1)	[72066]
		12536.61	(0.04)	2(0, 2)	- 1(0, 1)	[72066]
		13946.76	(0.04)	2(1, 1)	- 1(1, 0)	[72066]
$\text{C}(\text{CH}_2)^{13}\text{CHCHCHCH}$	25331.98	(0.04)	4(2, 3)	- 3(2, 2)	[72066]	
	11536.90	(0.04)	2(1, 2)	- 1(1, 1)	[72066]	
	12530.66	(0.04)	2(0, 2)	- 1(0, 1)	[72066]	
	13985.70	(0.04)	2(1, 1)	- 1(1, 0)	[72066]	
	17172.54	(0.04)	3(1, 3)	- 2(1, 2)	[72066]	
	22683.97	(0.04)	4(1, 4)	- 3(1, 3)	[72066]	
	23584.72	(0.04)	4(0, 4)	- 3(0, 3)	[72066]	
	25341.52	(0.04)	4(2, 3)	- 3(2, 2)	[72066]	
$\text{C}(\text{CH}_2)\text{CH}^{13}\text{CHCHCH}$	28664.54	(0.04)	5(0, 5)	- 4(0, 4)	[72066]	
	33700.84	(0.04)	6(0, 6)	- 5(0, 5)	[72066]	
	39424.30	(0.04)	6(1, 5)	- 5(1, 4)	[72066]	
	11440.80	(0.04)	2(1, 2)	- 1(1, 1)	[72066]	
	12415.19	(0.04)	2(0, 2)	- 1(0, 1)	[72066]	
	13809.20	(0.04)	2(1, 1)	- 1(1, 0)	[72066]	
	23457.24	(0.04)	4(0, 4)	- 3(0, 3)	[72066]	
	22523.53	(0.04)	4(1, 4)	- 3(1, 3)	[72066]	
$\text{C}(^{13}\text{CH}_2)\text{CHCHCHCH}$	25085.42	(0.04)	4(2, 3)	- 3(2, 2)	[72066]	
	33539.47	(0.04)	6(0, 5)	- 5(0, 5)	[72066]	
	39146.46	(0.04)	6(1, 5)	- 5(1, 4)	[72066]	
	11295.15	(0.04)	2(1, 2)	- 1(1, 1)	[72066]	
	12245.78	(0.04)	2(0, 2)	- 1(0, 1)	[72066]	
$\text{C}(\text{CH}_2)\text{CDCHCHCH}$	13577.60	(0.04)	2(1, 1)	- 1(1, 0)	[72066]	
	16832.04	(0.04)	3(1, 3)	- 2(1, 2)	[72066]	
	24723.45	(0.04)	4(2, 3)	- 3(2, 2)	[72066]	
	11400.44	(0.04)	2(1, 2)	- 1(1, 1)	[72066]	
	12400.18	(0.04)	2(0, 2)	- 1(0, 1)	[72066]	
	13936.26	(0.04)	2(1, 1)	- 1(1, 0)	[72066]	
	16947.58	(0.04)	3(1, 3)	- 2(1, 2)	[72066]	
	18000.48	(0.04)	3(0, 3)	- 2(0, 2)	[72066]	
	20004.59	(0.04)	3(2, 1)	- 2(2, 0)	[72066]	
	23162.90	(0.04)	4(0, 4)	- 3(0, 3)	[72066]	
	22356.23	(0.04)	4(1, 4)	- 3(1, 3)	[72066]	
	25125.72	(0.04)	4(2, 3)	- 3(2, 2)	[72066]	
$\text{C}(\text{CH}_2)\text{CHCDCHCH}$	20945.05	(0.04)	4(2, 3)	- 4(0, 4)	[72066]	
	23898.11	(0.04)	5(2, 4)	- 5(0, 5)	[72066]	
	28124.01	(0.04)	5(0, 5)	- 4(0, 4)	[72066]	
	11177.38	(0.04)	2(1, 2)	- 1(1, 1)	[72066]	
	12126.91	(0.04)	2(0, 2)	- 1(0, 1)	[72066]	
	13478.73	(0.04)	2(1, 1)	- 1(1, 0)	[72066]	
	16649.68	(0.04)	3(1, 3)	- 2(1, 2)	[72066]	
	17725.04	(0.04)	3(0, 3)	- 2(0, 2)	[72066]	
	19259.02	(0.04)	3(2, 1)	- 2(2, 0)	[72066]	
	22931.08	(0.04)	4(0, 4)	- 3(0, 3)	[72066]	
	22010.80	(0.04)	4(1, 4)	- 3(1, 3)	[72066]	
	24498.47	(0.04)	4(2, 3)	- 3(2, 2)	[72066]	
22079.68	(0.04)	4(2, 3)	- 4(0, 4)	[72066]		
24560.49	(0.04)	5(2, 4)	- 5(0, 5)	[72066]		
27893.34	(0.04)	5(0, 5)	- 4(0, 4)	[72066]		

TABLE 58.2. Microwave spectrum of 1-methylene-2,4-cyclopentadiene

C₆H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.	
C(CHD)CHCHCHCH	11090.69	(0.05)	2(1, 2) - 1(1, 1)	[73077]	
	13317.20	(0.05)	2(1, 1) - 1(1, 0)	[73077]	
	16529.76	(0.05)	3(1, 3) - 2(1, 2)	[73077]	
	18305.92	(0.05)	3(2, 2) - 2(2, 1)	[73077]	
	19007.41	(0.05)	3(2, 1) - 2(2, 0)	[73077]	
	19850.39	(0.05)	3(1, 2) - 2(1, 1)	[73077]	
	22814.29	(0.05)	4(0, 4) - 3(0, 3)	[73077]	
	24264.54	(0.05)	4(2, 3) - 3(2, 2)	[73077]	
	24723.52	(0.05)	4(3, 2) - 3(3, 1)	[73077]	
	24836.04	(0.05)	4(3, 1) - 3(3, 0)	[73077]	
	25856.35	(0.05)	4(2, 2) - 3(2, 1)	[73077]	
	22466.98	(0.05)	4(2, 3) - 4(0, 4)	[73077]	
	24797.51	(0.05)	5(2, 4) - 5(0, 5)	[73077]	
	C(CH ₂)CDCDCHCH	11001.52	(0.04)	2(1, 2) - 1(1, 1)	[72066]
		11962.04	(0.04)	2(0, 2) - 1(0, 1)	[72066]
		13417.91	(0.04)	2(1, 1) - 1(1, 0)	[72066]
		16360.54	(0.04)	3(1, 3) - 2(1, 2)	[72066]
17385.62		(0.04)	3(0, 3) - 2(0, 2)	[72066]	
19243.43		(0.04)	3(2, 1) - 2(2, 0)	[72066]	
18314.51		(0.04)	3(2, 2) - 2(2, 1)	[72066]	
19952.68		(0.04)	3(1, 2) - 2(1, 1)	[72066]	
22391.20		(0.04)	4(0, 4) - 3(0, 3)	[72066]	
21590.13		(0.04)	4(1, 4) - 3(1, 3)	[72066]	
24224.69		(0.04)	4(2, 3) - 3(2, 2)	[72066]	
24832.15		(0.04)	4(3, 2) - 3(3, 1)	[72066]	
20441.83		(0.04)	4(2, 3) - 4(0, 4)	[72066]	
17278.58	(0.04)	5(1, 4) - 5(1, 5)	[72066]		
27193.18	(0.04)	5(0, 5) - 4(0, 4)	[72066]		

Table 59.1. Molecular constants of bicyclo[2.2.0]hexa-2,5-diene (dewar benzene).

Parameter	Value
A (MHz)	7770.368(12)
B (MHz)	4479.287(9)
C (MHz)	3488.962(9)
<u>Electric Dipole Moment [74064]</u>	
μ_c (D)	0.0437

TABLE 59.2. Microwave spectrum of bicyclo[2.2.0]hexa-2,5-diene

C₆H₆


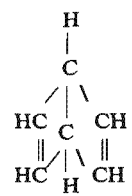
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
CHCHCHCHCHCH	20385.68	(0.10)	8(4, 5) - 8(3, 5)	[74064]
	21208.35	(0.10)	2(1, 1) - 1(0, 1)	[74064]
	26527.39	(0.10)	5(0, 5) - 4(1, 3)	[74064]
	26992.00	(0.10)	2(2, 0) - 1(1, 0)	[74064]
	27457.11	(0.10)	7(3, 4) - 7(2, 6)	[74064]
	27790.50	(0.10)	2(2, 1) - 1(1, 1)	[74064]
	28534.83	(0.10)	10(5, 6) - 10(4, 6)	[74064]
	30719.98	(0.10)	3(1, 2) - 2(0, 2)	[74064]
	30963.75	(0.10)	9(4, 5) - 9(3, 7)	[74064]
	31861.40	(0.10)	5(1, 4) - 4(2, 2)	[74064]
	34694.02	(0.10)	3(2, 1) - 2(1, 1)	[74064]
	36749.10	(0.10)	3(2, 2) - 2(1, 2)	[74064]
	40931.34	(0.10)	4(1, 3) - 3(0, 3)	[74064]
	42756.33	(0.10)	4(2, 2) - 3(1, 2)	[74064]
	42946.24	(0.10)	3(3, 1) - 2(2, 1)	[74064]

Table 60.1. Molecular constants for benzene-d₁.

Parameter	Value
<u>Rotational Analysis</u> [84031]	
A (MHz)	5689.144(6)
B (MHz)	5323.934(6)
C (MHz)	2749.674(6)
Δ_{JK} (MHz)	-0.0012(1)
Δ_K (MHz)	-0.0036(7)
δ_J (MHz)	0.000019
<u>Electric Dipole Moment</u> [87002]	
μ_a (D)	0.00810(28)

TABLE 60.2. Microwave spectrum of benzene-d

C₆H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
CDCHCHCHCHCH	8073.682	(0.065)	1(0, 1) - 0(0, 0)	[84031]
	8571.656	(0.009)	15(12, 3) - 15(12, 4)	[84031]
	8891.552	(0.015)	9(7, 2) - 9(7, 3)	[84031]
	8898.263	(0.009)	30(24, 6) - 30(24, 7)	[84031]
	9072.683	(0.033)	20(16, 4) - 20(16, 5)	[84031]
	10176.631	(0.015)	8(6, 3) - 8(6, 2)	[84031]
	10396.880	(0.036)	39(31, 8) - 39(31, 9)	[84031]
	10402.900	(0.032)	14(11, 3) - 14(11, 4)	[84031]
	10676.509	(0.097)	4(4, 1) - 4(2, 2)	[84031]
	11052.486	(0.036)	34(27, 7) - 34(27, 8)	[84031]
	11251.994	(0.008)	19(15, 4) - 19(15, 5)	[84031]
	11307.475	(0.039)	7(5, 2) - 7(5, 3)	[84031]
	11473.722	(0.014)	29(23, 6) - 29(23, 7)	[84031]
	11572.486	(0.027)	24(19, 5) - 24(19, 6)	[84031]
	12204.904	(0.037)	13(10, 3) - 13(10, 4)	[84031]
	12234.858	(0.053)	6(4, 3) - 6(4, 2)	[84031]
	13573.027	(0.024)	2(1, 2) - 1(1, 1)	[84031]
	13902.059	(0.024)	2(0, 2) - 1(0, 1)	[84031]
	14144.508	(0.057)	5(4, 2) - 5(2, 3)	[84031]
	14147.709	(0.019)	23(18, 5) - 23(18, 6)	[84031]

Table 61.1. Molecular constants of 1,3-cyclohexadiene.

Parameter	Ground State ^a	v=A [65031]	v=B [65031]
A'' (MHz)	5073.9995(92)	5069.50	5071.72
B'' (MHz)	5062.3483(59)	5055.20	5061.32
C'' (MHz)	2701.6929(40)	2695.80	2703.51
τ_1 (kHz)	-9.890(1008)		
τ_2 (kHz)	-2.794(335)		
τ_3^b (kHz)	6.700(380)		
τ_{aaaa} (kHz)	-5.98(50)		
τ_{bbbb} (kHz)	-4.247(406)		
τ_{cccc} (kHz)	-1.14(33)		
<u>Electric Dipole Moment [65031]</u>			
μ_a (D)	0.437(14)		

^aPresent work.^bValue fixed by setting $R_6 = 0$.

TABLE 61.2. Microwave spectrum of 1,3-cyclohexadiene

C₆H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
CHCHCHCHCH ₂ CH ₂	22622.95	(0.10)	2(2, 0) - 1(0, 1)	1 ν_{36}	[65031]
	23252.90	(0.10)	3(2, 2) - 2(2, 1)	1 ν_{36}	[65031]
	23295.45	(0.10)	3(1, 2) - 2(1, 1)	1 ν_{36}	[65031]
	23932.05	(0.10)	4(0, 4) - 3(0, 3)	1 ν_{36}	[65031]
	28665.70	(0.10)	4(2, 3) - 3(2, 2)	1 ν_{36}	[65031]
	28665.90	(0.10)	4(1, 3) - 3(1, 2)	1 ν_{36}	[65031]
	22634.30	(0.10)	2(2, 0) - 1(0, 1)	1 ν_{35}	[65031]
	23294.40	(0.10)	3(2, 2) - 2(2, 1)	1 ν_{35}	[65031]
	23325.40	(0.10)	3(1, 2) - 2(1, 1)	1 ν_{35}	[65031]
	23991.00	(0.10)	4(0, 4) - 3(0, 3)	1 ν_{35}	[65031]
	28717.20	(0.10)	4(2, 3) - 3(2, 2)	1 ν_{35}	[65031]

Table 62.1. Molecular constants for tricyclo[2.2.0.0^{2,6}]hexane.

Species	A (MHz)	B (MHz)	C (MHz)	Reference
Normal	5954.0715(26)	5256.3934(29)	4174.3995(34)	[present]
1- ¹³ C	5867.626(3)	5210.559(4)	4160.403(2)	[75051]
2- ¹³ C	5901.561(2)	5216.169(3)	4131.711(1)	[75051]
3- ¹³ C	5920.845(2)	5167.746(3)	4110.496(2)	[75051]
4- ¹³ C	5876.278(10)	5240.566(9)	4146.176(7)	[75051]
1-d ₁	5634.473(4)	5085.973(4)	4119.973(5)	[75051]
2-d ₁	5763.411(3)	5117.623(3)	4020.351(4)	[75051]
endo-3-d ₁	5762.491(2)	5077.017(2)	4069.970(2)	[75051]
exo-3-d ₁	5924.913(2)	5004.566(2)	4002.300(2)	[75051]
4-d ₁	5649.614(4)	5182.197(5)	4067.030(5)	[75051]
endo-3,5-d ₂	5553.196(11)	4938.978(14)	3968.920(7)	[75051]
<u>Electric Dipole Moment</u> [75051]				
μ _b (D)	0.089(4)			
μ _c (D)	0.2043(4)			

TABLE 62.2. Microwave spectrum of tricyclo[2.2.0.0(2,6)]hexane

C₆H₈

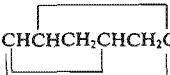
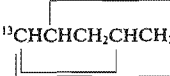
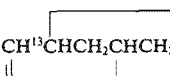
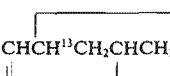
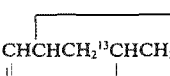
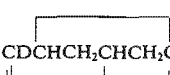
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.	
	11210.47	(0.05)	1(1, 0) - 0(0, 0)	[75051]	
	18477.29	(0.05)	2(1, 2) - 1(0, 1)	[75051]	
	21723.27	(0.05)	2(1, 1) - 1(0, 1)	[75051]	
	22036.64	(0.05)	2(2, 1) - 1(1, 0)	[75051]	
	22665.63	(0.05)	2(2, 0) - 1(1, 0)	[75051]	
	23118.63	(0.05)	2(2, 1) - 1(1, 1)	[75051]	
	23747.62	(0.05)	2(2, 0) - 1(1, 1)	[75051]	
	26285.98	(0.05)	3(0, 3) - 2(1, 2)	[75051]	
	32776.10	(0.05)	3(2, 1) - 2(1, 1)	[75051]	
	32801.95	(0.05)	3(1, 2) - 2(0, 2)	[75051]	
	33631.39	(0.05)	3(2, 2) - 2(1, 2)	[75051]	
	34460.81	(0.05)	3(3, 0) - 2(2, 0)	[75051]	
	34811.39	(0.05)	3(3, 1) - 2(2, 1)	[75051]	
	21499.33	(0.05)	2(1, 1) - 1(0, 1)	[75051]	
	22382.03	(0.05)	2(2, 0) - 1(1, 0)	[75051]	
	22813.46	(0.05)	2(2, 1) - 1(1, 1)	[75051]	
	32424.30	(0.05)	3(2, 1) - 2(1, 1)	[75051]	
	32465.33	(0.05)	3(1, 2) - 2(0, 2)	[75051]	
	33234.54	(0.05)	3(2, 2) - 2(1, 2)	[75051]	
	34003.75	(0.05)	3(3, 0) - 2(2, 0)	[75051]	
	34343.52	(0.05)	3(3, 1) - 2(2, 1)	[75051]	
	34594.71	(0.05)	4(0, 4) - 3(1, 3)	[75051]	
	34622.48	(0.05)	3(3, 0) - 2(2, 1)	[75051]	
	34656.58	(0.05)	4(1, 4) - 3(0, 3)	[75051]	
	22472.51	(0.05)	2(2, 0) - 1(1, 0)	[75051]	
	22920.86	(0.05)	2(2, 1) - 1(1, 1)	[75051]	
	32546.64	(0.05)	3(1, 2) - 2(0, 2)	[75051]	
	34159.73	(0.05)	3(3, 0) - 2(2, 0)	[75051]	
	34510.77	(0.05)	3(3, 1) - 2(2, 1)	[75051]	
	26032.88	(0.05)	3(0, 3) - 2(1, 2)	[75051]	
	34409.95	(0.05)	4(0, 4) - 3(1, 3)	[75051]	
	34475.47	(0.05)	4(1, 4) - 3(0, 3)	[75051]	
		22459.94	(0.05)	2(2, 0) - 1(1, 0)	[75051]
		22930.30	(0.05)	2(2, 1) - 1(1, 1)	[75051]
		32361.53	(0.05)	3(2, 1) - 2(1, 1)	[75051]
		32325.81	(0.05)	3(1, 2) - 2(0, 2)	[75051]
33265.76		(0.05)	3(2, 2) - 2(1, 2)	[75051]	
34205.72		(0.05)	3(3, 0) - 2(2, 0)	[75051]	
34548.62		(0.05)	3(3, 1) - 2(2, 1)	[75051]	
34315.42		(0.05)	4(1, 4) - 3(0, 3)	[75051]	
		21598.01	(0.05)	2(1, 1) - 1(0, 1)	[75051]
		22869.47	(0.05)	2(2, 1) - 1(1, 1)	[75051]
		32555.70	(0.05)	3(2, 1) - 2(1, 1)	[75051]
		32635.05	(0.05)	3(1, 2) - 2(0, 2)	[75051]
	33350.55	(0.05)	3(2, 2) - 2(1, 2)	[75051]	
	34417.82	(0.05)	3(3, 1) - 2(2, 1)	[75051]	
	26130.60	(0.05)	3(0, 3) - 2(1, 2)	[75051]	
	26382.55	(0.05)	3(1, 3) - 2(0, 2)	[75051]	
		20892.42	(0.05)	2(1, 1) - 1(0, 1)	[75051]
		21616.62	(0.05)	2(2, 0) - 1(1, 0)	[75051]
		21989.44	(0.05)	2(2, 1) - 1(1, 1)	[75051]
		31472.71	(0.05)	3(2, 1) - 2(1, 1)	[75051]
31551.71		(0.05)	3(1, 2) - 2(0, 2)	[75051]	
32161.32		(0.05)	3(2, 2) - 2(1, 2)	[75051]	
32770.94		(0.05)	3(3, 0) - 2(2, 0)	[75051]	
33080.80		(0.05)	3(3, 1) - 2(2, 1)	[75051]	
22582.62		(0.05)	2(2, 0) - 1(1, 1)	[75051]	
26039.08		(0.05)	3(1, 3) - 2(0, 2)	[75051]	
21116.31		(0.05)	2(1, 1) - 1(0, 1)	[75051]	
21974.40		(0.05)	2(2, 0) - 1(1, 0)	[75051]	
22407.87	(0.05)	2(2, 1) - 1(1, 1)	[75051]		
31837.55	(0.05)	3(2, 1) - 2(1, 1)	[75051]		
31911.14	(0.05)	3(1, 2) - 2(0, 2)	[75051]		
32643.09	(0.05)	3(2, 2) - 2(1, 2)	[75051]		
33375.04	(0.05)	3(3, 0) - 2(2, 0)	[75051]		
33728.35	(0.05)	3(3, 1) - 2(2, 1)	[75051]		

TABLE 62.2. Microwave spectrum of tricyclo[2.2.0.0(2,6)]hexane — Continued

C₆H

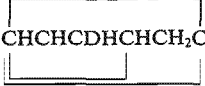
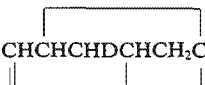
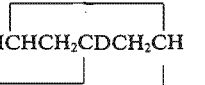
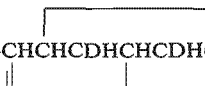
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
	23071.67	(0.05)	2(2, 0) - 1(1, 1)	[75051]
	25379.15	(0.05)	3(0, 3) - 2(1, 2)	[75051]
	20993.57	(0.05)	2(1, 1) - 1(0, 1)	[75051]
	21928.58	(0.05)	2(2, 0) - 1(1, 0)	[75051]
	22364.51	(0.05)	2(2, 1) - 1(1, 1)	[75051]
	31687.42	(0.05)	3(2, 1) - 2(1, 1)	[75051]
	31681.37	(0.05)	3(1, 2) - 2(0, 2)	[75051]
	32518.51	(0.05)	3(2, 2) - 2(1, 2)	[75051]
	33355.66	(0.05)	3(3, 0) - 2(2, 0)	[75051]
	33682.37	(0.05)	3(3, 1) - 2(2, 1)	[75051]
	25572.49	(0.05)	3(0, 3) - 2(1, 2)	[75051]
	25883.52	(0.05)	3(1, 3) - 2(0, 2)	[75051]
	20938.62	(0.05)	2(1, 1) - 1(0, 1)	[75051]
	22265.18	(0.05)	2(2, 0) - 1(1, 0)	[75051]
	22779.30	(0.05)	2(2, 1) - 1(1, 1)	[75051]
	31750.17	(0.05)	3(2, 1) - 2(1, 1)	[75051]
	31508.59	(0.05)	3(1, 2) - 2(0, 2)	[75051]
	32788.42	(0.05)	3(2, 2) - 2(1, 2)	[75051]
	34068.26	(0.05)	3(3, 0) - 2(2, 0)	[75051]
	34385.38	(0.05)	3(3, 1) - 2(2, 1)	[75051]
	23267.44	(0.05)	2(2, 0) - 1(1, 1)	[75051]
	25133.99	(0.05)	3(0, 3) - 2(1, 2)	[75051]
	21196.24	(0.05)	2(1, 1) - 1(0, 1)	[75051]
	21782.48	(0.05)	2(2, 0) - 1(1, 0)	[75051]
	22131.05	(0.05)	2(2, 1) - 1(1, 1)	[75051]
	31880.78	(0.05)	3(2, 1) - 2(1, 1)	[75051]
	32495.40	(0.05)	3(2, 2) - 2(1, 2)	[75051]
	32927.67	(0.05)	3(3, 0) - 2(2, 0)	[75051]
	33263.38	(0.05)	3(3, 1) - 2(2, 1)	[75051]
	21015.91	(0.05)	2(2, 1) - 1(1, 0)	[75051]
	25664.58	(0.05)	3(0, 3) - 2(1, 2)	[75051]
	20370.11	(0.05)	2(1, 1) - 1(0, 1)	[75051]
	20628.51	(0.05)	2(2, 0) - 1(1, 0)	[75051]
	21598.60	(0.05)	2(2, 1) - 1(1, 1)	[75051]
	22167.08	(0.05)	2(2, 0) - 1(1, 1)	[75051]
	24925.08	(0.05)	3(0, 3) - 2(1, 2)	[75051]
	25187.13	(0.05)	3(1, 3) - 2(0, 2)	[75051]

Table 63.1. Molecular constants of bicyclo[2.1.1]hex-2-ene.

Species	A (MHz)	B (MHz)	C (MHz)	Reference
Normal	5820.66(12)	4689.6060(67)	4289.5905(66)	[present]
1- ¹³ C	5752.524(103)	4685.847(6)	4249.150(7)	[76054]
2- ¹³ C	5792.950(58)	4627.840(3)	4223.050(3)	[76054]
5- ¹³ C	5748.483(79)	4612.760(4)	4264.360(4)	[76054]
<u>Dipole Moment</u> [76054]				
μ_a (D)	0.299(8)			

TABLE 63.2. Microwave Spectrum Of bicyclo[2.1.1]hex-2-ene

C₆H₈

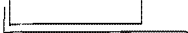
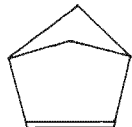
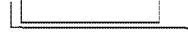


Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.	
$\text{CHCHCHCH}(\text{CH}_2)\text{CH}_2$  	8979.22	(0.05)	1(0, 1) - 0(0, 0)	[76054]	
	17558.43	(0.05)	2(1, 2) - 1(1, 1)	[76054]	
	17869.75	(0.05)	2(0, 2) - 1(0, 1)	[76054]	
	26287.22	(0.05)	3(1, 3) - 2(1, 2)	[76054]	
	26608.32	(0.05)	3(0, 3) - 2(0, 2)	[76054]	
	26937.62	(0.05)	3(2, 2) - 2(2, 1)	[76054]	
	27266.94	(0.05)	3(2, 1) - 2(2, 0)	[76054]	
	27474.58	(0.05)	3(1, 2) - 2(1, 1)	[76054]	
	34970.94	(0.05)	4(1, 4) - 3(1, 3)	[76054]	
	35209.55	(0.05)	4(0, 4) - 3(0, 3)	[76054]	
	35846.92	(0.05)	4(2, 3) - 3(2, 2)	[76054]	
	36062.51	(0.05)	4(3, 2) - 3(3, 1)	[76054]	
	36135.85	(0.05)	4(3, 1) - 3(3, 0)	[76054]	
	36497.70	(0.05)	4(1, 3) - 3(1, 2)	[76054]	
	36552.66	(0.05)	4(2, 2) - 3(2, 1)	[76054]	
$^{13}\text{CHCHCHCH}(\text{CH}_2)\text{CH}_2$ 	26805.03	(0.05)	3(2, 2) - 2(2, 1)	[76054]	
	27202.58	(0.05)	3(2, 1) - 2(2, 0)	[76054]	
	27381.03	(0.05)	3(1, 2) - 2(1, 1)	[76054]	
	34691.52	(0.05)	4(1, 4) - 3(1, 3)	[76054]	
	34909.14	(0.05)	4(0, 4) - 3(0, 3)	[76054]	
	35653.86	(0.05)	4(2, 3) - 3(2, 2)	[76054]	
	35915.06	(0.05)	4(3, 2) - 3(3, 1)	[76054]	
	36016.29	(0.05)	4(3, 1) - 3(3, 0)	[76054]	
	36337.05	(0.05)	4(1, 3) - 3(1, 2)	[76054]	
	36482.44	(0.05)	4(2, 2) - 3(2, 1)	[76054]	
$\text{CH}^{13}\text{CHCHCH}(\text{CH}_2)\text{CH}_2$ 	26552.67	(0.05)	3(2, 2) - 2(2, 1)	[76054]	
	26881.73	(0.05)	3(2, 1) - 2(2, 0)	[76054]	
	27097.11	(0.05)	3(1, 2) - 2(1, 1)	[76054]	
	34448.23	(0.05)	4(1, 4) - 3(1, 3)	[76054]	
	34694.71	(0.05)	4(0, 4) - 3(0, 3)	[76054]	
	35333.93	(0.05)	4(2, 3) - 3(2, 2)	[76054]	
	35549.31	(0.05)	4(3, 2) - 3(3, 1)	[76054]	
	35621.40	(0.05)	4(3, 1) - 3(3, 0)	[76054]	
	35995.29	(0.05)	4(1, 3) - 3(1, 2)	[76054]	
	36041.36	(0.05)	4(2, 2) - 3(2, 1)	[76054]	
	$\text{CHCHCHCH}(\text{CH}_2)^{13}\text{CH}_2$ 	26331.39	(0.05)	3(2, 2) - 2(2, 1)	[76054]
		26889.86	(0.05)	3(2, 1) - 2(2, 0)	[76054]
27105.98		(0.05)	3(1, 2) - 2(1, 1)	[76054]	
34696.55		(0.05)	4(1, 4) - 3(1, 3)	[76054]	
34939.64		(0.05)	4(0, 4) - 3(0, 3)	[76054]	
35454.62		(0.05)	4(2, 3) - 3(2, 2)	[76054]	
35623.57		(0.05)	4(3, 2) - 3(3, 1)	[76054]	
35674.05		(0.05)	4(3, 1) - 3(3, 0)	[76054]	
36039.67		(0.05)	4(1, 3) - 3(1, 2)	[76054]	
36022.55		(0.05)	4(2, 2) - 3(2, 1)	[76054]	

Table 64.1. Molecular constants of bicyclo[3.1.0]hex-2-ene.

Species	A(MHz)	B (MHz)	C(MHz)	Reference
Normal	6306.121(66)	4516.6670(43)	3208.8226(18)	[present]
1- ¹³ C	6249.016(4)	4489.502(4)	3187.593(1)	[78030]
2- ¹³ C	6200.995(8)	4498.162(36)	3172.108(4)	[78030]
5- ¹³ C	6249.495(26)	4492.845(10)	3188.046(4)	[78030]
6- ¹³ C	6276.204(55)	4418.036(24)	3166.229(5)	[78030]
<u>Electric Dipole Moment</u> [78030]				
μ_a (D)	0.166(9)			
μ_b (D)	0.209(15)			
μ_c (D)	0.119(1)			

TABLE 64.2. Microwave spectrum of bicyclo[3.1.0]hex-2-ene

C₆H₈


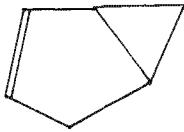
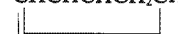


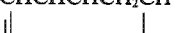
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.	
$\text{CHCHCHCH}_2\text{CHCH}_2$  	20543.37	(0.05)	3(0, 3) - 2(1, 2)	[78030]	
	20944.57	(0.05)	3(1, 3) - 2(1, 2)	[78030]	
	21925.66	(0.05)	3(1, 3) - 2(0, 2)	[78030]	
	22626.70	(0.05)	2(2, 0) - 1(1, 0)	[78030]	
	23176.48	(0.05)	3(2, 2) - 2(2, 1)	[78030]	
	23934.52	(0.05)	2(2, 0) - 1(1, 1)	[78030]	
	24828.47	(0.05)	3(2, 1) - 2(2, 0)	[78030]	
	27426.52	(0.05)	4(0, 4) - 3(1, 3)	[78030]	
	27561.67	(0.05)	4(1, 4) - 3(1, 3)	[78030]	
	27827.70	(0.05)	4(0, 4) - 3(0, 3)	[78030]	
	27962.82	(0.05)	4(1, 4) - 3(0, 3)	[78030]	
	$^{13}\text{CHCHCHCH}_2\text{CHCH}_2$ 	27249.12	(0.05)	4(0, 4) - 3(1, 3)	[78030]
		27379.03	(0.05)	4(1, 4) - 3(1, 3)	[78030]
		27638.03	(0.05)	4(0, 4) - 3(0, 3)	[78030]
28158.33		(0.05)	4(1, 3) - 3(2, 2)	[78030]	
33796.86		(0.05)	5(0, 5) - 4(1, 4)	[78030]	
33835.75		(0.05)	5(1, 5) - 4(1, 4)	[78030]	
33926.77		(0.05)	5(0, 5) - 4(0, 4)	[78030]	
33965.66		(0.05)	5(1, 5) - 4(0, 4)	[78030]	
34853.23		(0.05)	3(3, 1) - 2(2, 0)	[78030]	
35486.42		(0.05)	3(3, 0) - 2(2, 1)	[78030]	
$\text{CH}^{13}\text{CHCHCH}_2\text{CHCH}_2$ 	27157.68	(0.05)	4(0, 4) - 3(1, 3)	[78030]	
	27272.11	(0.05)	4(1, 4) - 3(1, 3)	[78030]	
	27512.46	(0.05)	4(0, 4) - 3(0, 3)	[78030]	
	27626.91	(0.05)	4(1, 4) - 3(0, 3)	[78030]	
	33659.73	(0.05)	5(0, 5) - 4(1, 4)	[78030]	
	33692.81	(0.05)	5(1, 5) - 4(1, 4)	[78030]	
	33774.18	(0.05)	5(0, 5) - 4(0, 4)	[78030]	
	33802.25	(0.05)	4(2, 3) - 3(1, 2)	[78030]	
	33807.27	(0.05)	5(1, 5) - 4(0, 4)	[78030]	
	34596.45	(0.05)	3(3, 1) - 2(2, 0)	[78030]	
$\text{CHCHCHCH}_2^{13}\text{CHCH}_2$ 	27256.66	(0.05)	4(0, 4) - 3(1, 3)	[78030]	
	27385.46	(0.05)	4(1, 4) - 3(1, 3)	[78030]	
	27643.33	(0.05)	4(0, 4) - 3(0, 3)	[78030]	
	27772.13	(0.05)	4(1, 4) - 3(0, 3)	[78030]	
	28182.02	(0.05)	4(1, 3) - 3(2, 2)	[78030]	
	33368.64	(0.05)	4(2, 2) - 3(2, 1)	[78030]	
	33804.44	(0.05)	5(0, 5) - 4(1, 4)	[78030]	
	33842.73	(0.05)	5(1, 5) - 4(1, 4)	[78030]	
	33933.25	(0.05)	5(0, 5) - 4(0, 4)	[78030]	
	33971.54	(0.05)	5(1, 5) - 4(0, 4)	[78030]	
$\text{CHCHCHCH}_2\text{CH}^{13}\text{CH}_2$ 	34034.73	(0.05)	4(2, 3) - 3(1, 2)	[78030]	
	20172.83	(0.05)	3(0, 3) - 2(1, 2)	[78030]	
	27004.81	(0.05)	4(0, 4) - 3(1, 3)	[78030]	
	27166.98	(0.05)	4(1, 4) - 3(1, 3)	[78030]	
	27460.89	(0.05)	4(0, 4) - 3(0, 3)	[78030]	
	27623.09	(0.05)	4(1, 4) - 3(0, 3)	[78030]	
	33538.46	(0.05)	5(0, 5) - 4(1, 4)	[78030]	
	33590.05	(0.05)	5(1, 5) - 4(1, 4)	[78030]	
33700.68	(0.05)	5(0, 5) - 4(0, 4)	[78030]		
33752.26	(0.05)	5(1, 5) - 4(0, 4)	[78030]		

Table 65.1. Molecular constants of
1,2-dimethylene cyclobutane.

Parameter	Ground State
A'' (MHz)	4925.1758(49)
B'' (MHz)	4089.9668(102)
C'' (MHz)	2301.6881(46)
τ_1 (kHz)	3.77(71)
τ_2 (kHz)	0 ^a
τ_3^b (kHz)	-55.(32)
τ_{aaaa} (kHz)	0 ^a
τ_{bbbb} (kHz)	-8.10(108)
τ_{cccc} (kHz)	-0.64(21)
μ_b (D)	0.457(2)

^aFixed at 0.^bValue determined by setting $R_g = 0$.Table 65.2. Molecular constants of vibrational states of
1,2-dimethylene cyclobutane. [75052]

Vibrational State	v	A (MHz)	B (MHz)	C (MHz)
<u>C(CH₂)C(CH₂)CH₂CH₂</u>				
	1	4930.092	4080.071	2308.365
	2	4934.096	4071.403	2313.958
	3	4937.205	4064.896	2318.945
	4	4939.677	4059.131	2323.442

TABLE 65.3. Microwave spectrum of 1,2-dimethylene cyclobutane

C₆H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$	$- J''(K_{-1}, K_{+1})$	Vib. state	Ref.
C(CH ₂)C(CH ₂)CH ₂ CH ₂	27243.00	(0.05)	3(3, 1)	- 2(2, 0)		[75052]
	29057.33	(0.05)	3(3, 0)	- 2(2, 1)		[75052]
	29378.76	(0.05)	5(1, 4)	- 4(2, 3)		[75052]
H ₂ C=C-C=CH ₂ H ₂ C-CH ₂	29712.50	(0.05)	5(2, 4)	- 4(1, 3)		[75052]
	29786.63	(0.05)	6(0, 6)	- 5(1, 5)		[75052]
	29787.59	(0.05)	6(1, 6)	- 5(0, 5)		[75052]
	31961.11	(0.05)	4(3, 2)	- 3(2, 1)		[75052]
	34102.30	(0.05)	6(1, 5)	- 5(2, 4)		[75052]
	34165.86	(0.05)	6(2, 5)	- 5(1, 4)		[75052]
	34389.98	(0.05)	7(1, 7)	- 6(0, 6)		[75052]
	34389.98	(0.05)	7(0, 7)	- 6(1, 6)		[75052]
	35651.13	(0.05)	5(3, 3)	- 4(2, 2)		[75052]
	37464.33	(0.05)	4(4, 1)	- 3(3, 0)		[75052]
	37923.05	(0.05)	6(2, 4)	- 5(3, 3)		[75052]
	38375.97	(0.05)	4(4, 0)	- 3(3, 1)		[75052]
	38397.53	(0.05)	6(3, 3)	- 5(4, 2)		[75052]
	38725.45	(0.05)	7(1, 6)	- 6(2, 5)		[75052]
	38735.90	(0.05)	7(2, 6)	- 6(1, 5)		[75052]
	38993.08	(0.05)	8(0, 8)	- 7(1, 7)		[75052]
	38993.08	(0.05)	8(1, 8)	- 7(0, 7)		[75052]
	39191.16	(0.05)	6(3, 4)	- 5(2, 3)		[75052]
	39273.41	(0.05)	4(3, 1)	- 3(2, 2)		[75052]
	27277.48	(0.05)	3(3, 1)	- 2(2, 0)	1ν ₃₆	[75052]
	29048.92	(0.05)	3(3, 0)	- 2(2, 1)	1ν ₃₆	[75052]
	38384.65	(0.05)	4(4, 0)	- 3(3, 1)	1ν ₃₆	[75052]
	37506.90	(0.05)	4(4, 1)	- 3(3, 0)	1ν ₃₆	[75052]
	32012.80	(0.05)	4(3, 2)	- 3(2, 1)	1ν ₃₆	[75052]
	35721.48	(0.05)	5(3, 3)	- 4(2, 2)	1ν ₃₆	[75052]
	29403.93	(0.05)	5(1, 4)	- 4(2, 3)	1ν ₃₆	[75052]
	29758.94	(0.05)	5(2, 4)	- 4(1, 3)	1ν ₃₆	[75052]
	38288.33	(0.05)	6(3, 3)	- 5(4, 2)	1ν ₃₆	[75052]
	37913.90	(0.05)	6(2, 4)	- 5(3, 3)	1ν ₃₆	[75052]
	39258.05	(0.05)	6(3, 4)	- 5(2, 3)	1ν ₃₆	[75052]
	34148.35	(0.05)	6(1, 5)	- 5(2, 4)	1ν ₃₆	[75052]
	34217.55	(0.05)	6(2, 5)	- 5(1, 4)	1ν ₃₆	[75052]
	29856.15	(0.05)	6(0, 6)	- 5(1, 5)	1ν ₃₆	[75052]
	29857.25	(0.05)	6(1, 6)	- 5(0, 5)	1ν ₃₆	[75052]
	38798.31	(0.05)	7(2, 6)	- 6(1, 5)	1ν ₃₆	[75052]
	38786.79	(0.05)	7(1, 6)	- 6(2, 5)	1ν ₃₆	[75052]
	34472.98	(0.05)	7(1, 7)	- 6(0, 6)	1ν ₃₆	[75052]
	34472.98	(0.05)	7(0, 7)	- 6(1, 6)	1ν ₃₆	[75052]
	39089.56	(0.05)	8(0, 8)	- 7(1, 7)	1ν ₃₆	[75052]
	39089.56	(0.05)	8(1, 8)	- 7(0, 7)	1ν ₃₆	[75052]
	27305.62	(0.05)	3(3, 1)	- 2(2, 0)	2ν ₃₆	[75052]
	29040.85	(0.05)	3(3, 0)	- 2(2, 1)	2ν ₃₆	[75052]
	38391.10	(0.05)	4(4, 0)	- 3(3, 1)	2ν ₃₆	[75052]
	37541.57	(0.05)	4(4, 1)	- 3(3, 0)	2ν ₃₆	[75052]
	32055.68	(0.05)	4(3, 2)	- 3(2, 1)	2ν ₃₆	[75052]
	35780.56	(0.05)	5(3, 3)	- 4(2, 2)	2ν ₃₆	[75052]
	29423.35	(0.05)	5(1, 4)	- 4(2, 3)	2ν ₃₆	[75052]
	29797.40	(0.05)	5(2, 4)	- 4(1, 3)	2ν ₃₆	[75052]
	38077.17	(0.05)	6(3, 3)	- 5(4, 2)	2ν ₃₆	[75052]
	37901.90	(0.05)	6(2, 4)	- 5(3, 3)	2ν ₃₆	[75052]
	39314.47	(0.05)	6(3, 4)	- 5(2, 3)	2ν ₃₆	[75052]
	34185.56	(0.05)	6(1, 5)	- 5(2, 4)	2ν ₃₆	[75052]
	34259.73	(0.05)	6(2, 5)	- 5(1, 4)	2ν ₃₆	[75052]
	29913.98	(0.05)	6(0, 6)	- 5(1, 5)	2ν ₃₆	[75052]
	29915.13	(0.05)	6(1, 6)	- 5(0, 5)	2ν ₃₆	[75052]
	38849.56	(0.05)	7(2, 6)	- 6(1, 5)	2ν ₃₆	[75052]
	38836.94	(0.05)	7(1, 6)	- 6(2, 5)	2ν ₃₆	[75052]
	34541.95	(0.05)	7(1, 7)	- 6(0, 6)	2ν ₃₆	[75052]
	34541.95	(0.05)	7(0, 7)	- 6(1, 6)	2ν ₃₆	[75052]
	39169.62	(0.05)	8(0, 8)	- 7(1, 7)	2ν ₃₆	[75052]
	39169.62	(0.05)	8(1, 8)	- 7(0, 7)	2ν ₃₆	[75052]
	27328.20	(0.05)	3(3, 1)	- 2(2, 0)	3ν ₃₆	[75052]
	38396.65	(0.05)	4(4, 0)	- 3(3, 1)	3ν ₃₆	[75052]
	32090.77	(0.05)	4(3, 2)	- 3(2, 1)	3ν ₃₆	[75052]
	29832.33	(0.05)	5(2, 4)	- 4(1, 3)	3ν ₃₆	[75052]

TABLE 65.3. Microwave spectrum of 1,2-dimethylene cyclobutane — Continued

C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	37896.17	(0.05)	6(2, 4) - 5(3, 3)	3ν ₃₆	[75052]
	34298.88	(0.05)	6(2, 5) - 5(1, 4)	3ν ₃₆	[75052]
	29965.88	(0.05)	6(0, 6) - 5(1, 5)	3ν ₃₆	[75052]
	29967.11	(0.05)	6(1, 6) - 5(0, 5)	3ν ₃₆	[75052]
	38883.26	(0.05)	7(1, 6) - 6(2, 5)	3ν ₃₆	[75052]
	34604.03	(0.05)	7(1, 7) - 6(0, 6)	3ν ₃₆	[75052]
	34604.03	(0.05)	7(0, 7) - 6(1, 6)	3ν ₃₆	[75052]
	39241.76	(0.05)	8(0, 8) - 7(1, 7)	3ν ₃₆	[75052]
	39241.76	(0.05)	8(1, 8) - 7(0, 7)	3ν ₃₆	[75052]
	27346.50	(0.05)	3(3, 1) - 2(2, 0)	4ν ₃₆	[75052]
	29028.53	(0.05)	3(3, 0) - 2(2, 1)	4ν ₃₆	[75052]
	38400.20	(0.05)	4(4, 0) - 3(3, 1)	4ν ₃₆	[75052]
	32120.80	(0.05)	4(3, 2) - 3(2, 1)	4ν ₃₆	[75052]
	29460.20	(0.05)	5(1, 4) - 4(2, 3)	4ν ₃₆	[75052]
	29863.30	(0.05)	5(2, 4) - 4(1, 3)	4ν ₃₆	[75052]
	34333.55	(0.05)	6(2, 5) - 5(1, 4)	4ν ₃₆	[75052]
	30012.60	(0.05)	6(0, 6) - 5(1, 5)	4ν ₃₆	[75052]
	30013.92	(0.05)	6(1, 6) - 5(0, 5)	4ν ₃₆	[75052]
	34659.93	(0.05)	7(1, 7) - 6(0, 6)	4ν ₃₆	[75052]
	34659.93	(0.05)	7(0, 7) - 6(1, 6)	4ν ₃₆	[75052]
	39306.75	(0.05)	8(0, 8) - 7(1, 7)	4ν ₃₆	[75052]
	39306.75	(0.05)	8(1, 8) - 7(0, 7)	4ν ₃₆	[75052]

Table 66.1. Molecular constants for t-butyl acetylene.

Species	B ₀ (MHz)	C ₀ (MHz)
<u>Ground State</u> [62022]		
(CH ₃) ₃ CC≡CH	2683.18(1)	----
(CH ₃) ₃ CC≡ ¹³ CH	2609.35(2)	----
(CH ₃) ₃ C ¹³ C≡CH	2665.90(2)	----
(CH ₃) ₃ CC≡CD	2531.09(2)	----
(CH ₃) ₃ CC≡ ¹³ CD	2467.53(2)	----
(CH ₃) ₃ C ¹³ C≡CD	2516.83(2)	----
¹³ CH ₃ (CH ₃) ₂ CC≡CH	2672.45(3)	2643.36(3)
¹³ CH ₃ (CH ₃) ₂ CC≡CD	2520.65(3)	2494.72(3)
<u>Excited States of (CH₃)₃CC≡CH</u> [62022]		
<u>v State</u>	<u>B_v (MHz)</u>	<u>q_g (MHz)</u>
T _e ^a	2681.67	1.90
T _a	2682.05	----
B _e ^b	2685.77	3.37

^aTorsional state.^bSkeletal bending mode.

TABLE 66.2. Microwave spectrum of tertiary butyl acetylene

C₆H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
(CH ₃) ₃ CCCH	10732.9	(0.1)	2() - 1()		[62022]
	16099.3	(0.1)	3() - 2()		[62022]
	21446.0	(0.1)	4(-1) - 3(-1)	1ν _{Tc} ℓ = -1	[62022]
	21453.5	(0.1)	4() - 3()	1ν _{Tc}	[62022]
	21456.4	(0.1)	4() - 3()	1ν _{Ta}	[62022]
	21465.5	(0.1)	4() - 3()		[60008]
	21486.4	(0.1)	4() - 3()	1ν _{Be}	[62022]
	21499.7	(0.1)	4(1) - 3(1)	1ν _{Be} ℓ = +1	[62022]
	26807.3	(0.1)	5(-1) - 4(-1)	1ν _{Tc} ℓ = -1	[62022]
	26816.8	(0.1)	5() - 4()	1ν _{Tc}	[62022]
	26820.4	(0.1)	5() - 4()	1ν _{Ta}	[62022]
	26831.9	(0.1)	5() - 4()		[62022]
	26857.7	(0.1)	5() - 4()	1ν _{Be}	[62022]
	26874.5	(0.1)	5(1) - 4(1)	1ν _{Be} ℓ = +1	[62022]
	32168.4	(0.1)	6(-1) - 5(-1)	1ν _{Tc} ℓ = -1	[62022]
	32179.8	(0.1)	6() - 5()	1ν _{Tc}	[62022]
	32184.3	(0.1)	6() - 5()	1ν _{Ta}	[62022]
	32198.0	(0.1)	6() - 5()		[62022]
	32229.0	(0.1)	6() - 5()	1ν _{Be}	[62022]
	32249.5	(0.1)	6(-1) - 5(-1)	1ν _{Be} ℓ = -1	[62022]
CH ₃) ₂ CC ¹³ CH	20874.9	(0.1)	4() - 3()		[62022]
	26093.5	(0.1)	5() - 4()		[62022]
	31312.1	(0.1)	6() - 5()		[62022]
(CH ₃) ₃ C ¹³ CCH	21327.2	(0.1)	4() - 3()		[62022]
	26659.1	(0.1)	5() - 4()		[62022]
(CH ₃) ₃ CCCD	31990.5	(0.1)	6() - 5()		[62022]
	20248.8	(0.1)	4() - 3()		[60008]
	25310.9	(0.1)	5() - 4()		[60008]
(CH ₃) ₃ CC ¹³ CD	30373.0	(0.1)	6() - 5()		[62022]
	19740.3	(0.1)	4() - 3()		[62022]
	24675.4	(0.1)	5() - 4()		[62022]
(CH ₃) ₃ C ¹³ CCD	29610.2	(0.1)	6() - 5()		[62022]
	20134.6	(0.1)	4() - 3()		[62022]
	25168.2	(0.1)	5() - 4()		[62022]
¹³ CH ₃ (CH ₃) ₂ CCCH	30201.9	(0.1)	6() - 5()		[62022]
	21204.4	(0.1)	4(1, 4) - 3(1, 3)		[62022]
	21320.8	(0.1)	4(1, 3) - 3(1, 2)		[62022]
	26504.7	(0.1)	5(1, 5) - 4(1, 4)		[62022]
	26650.1	(0.1)	5(1, 4) - 4(1, 3)		[62022]
	31804.5	(0.1)	6(1, 6) - 5(1, 5)		[62022]
¹³ CH ₃ (CH ₃) ₂ CCCD	31979.1	(0.1)	6(1, 5) - 5(1, 4)		[62022]
	20009.0	(0.1)	4(1, 4) - 3(1, 3)		[62022]
	20112.4	(0.1)	4(1, 3) - 3(1, 2)		[62022]
	25010.9	(0.1)	5(1, 5) - 4(1, 4)		[62022]
	25140.6	(0.1)	5(1, 4) - 4(1, 3)		[62022]
	30012.2	(0.1)	6(1, 6) - 5(1, 5)		[62022]
	30167.8	(0.1)	6(1, 5) - 5(1, 4)		[62022]

Table 67.1. Molecular constants of cyclohexene.

Parameter	Normal ^a Ground State	Parameter	Normal $\nu_{4,2} = 1^b$	3,3,6,6-d ₄ ^b	C ₆ D ₁₀ ^b
A'' (MHz)	4739.1678(115)	A	4733.11	4601.95	3723.97
B'' (MHz)	4544.426(12)	B	4544.88	3806.39	3523.13
C'' (MHz)	2562.415(6)	C	2562.39	2342.66	2071.02
τ_1 (kHz)	-10.5(34)				
τ_2 (kHz)	-3.23(1.12)				
τ_3^c (kHz)	312.(64)				
τ_{aaaa} (kHz)	-7.0(18)				
τ_{bbbb} (kHz)	-3.9(16)				
τ_{cccc} (kHz)	-1.7(8)				
μ_b (D)	0.331(2) ^b				

^aThis work.^b[68046]^cValue fixed by setting $R_6 = 0$.

TABLE 67.2. Microwave spectrum of cyclohexene

C₆H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
CHCHCH ₂ CH ₂ CH ₂ CH ₂	7301.56	(0.10)	1(1, 1) - 0(0, 0)		[69061]
	7745.10	(0.10)	5(5, 1) - 5(4, 2)		[69061]
	10074.04	(0.10)	5(3, 2) - 5(2, 3)		[69061]
	10244.93	(0.10)	4(2, 2) - 4(1, 3)		[69061]
	10337.85	(0.10)	3(1, 2) - 3(0, 3)		[69061]
	10405.23	(0.10)	3(2, 2) - 3(1, 3)		[69061]
	10512.48	(0.08)	5(4, 2) - 5(3, 3)		[68046]
	10633.04	(0.08)	6(5, 2) - 6(4, 3)		[68046]
	12217.99	(0.08)	2(0, 2) - 1(1, 1)		[68046]
	12420.28	(0.08)	2(1, 2) - 1(0, 1)	1ν ₄₂	[68046]
	12426.39	(0.08)	2(1, 2) - 1(0, 1)		[68046]
	14491.55	(0.08)	8(6, 3) - 8(5, 4)		[68046]
	14496.07	(0.08)	7(5, 3) - 7(4, 4)		[68046]
	14505.14	(0.08)	5(2, 3) - 5(1, 4)		[68046]
	14508.32	(0.08)	6(4, 3) - 6(3, 4)		[68046]
	14521.62	(0.08)	5(3, 3) - 5(2, 4)		[68046]
	14528.38	(0.10)	4(1, 3) - 4(0, 4)		[69061]
	14532.32	(0.08)	4(2, 3) - 4(1, 4)		[68046]
	16761.73	(0.08)	2(2, 1) - 1(1, 0)	1ν ₄₂	[68046]
	16779.86	(0.08)	2(2, 1) - 1(1, 0)		[68046]
	17442.66	(0.08)	3(0, 3) - 2(1, 2)	1ν ₄₂	[68046]
	17444.97	(0.08)	3(0, 3) - 2(1, 2)		[68046]
	17456.05	(0.08)	3(1, 3) - 2(0, 2)	1ν ₄₂	[68046]
	17459.27	(0.08)	3(1, 3) - 2(0, 2)		[68046]
	20551.44	(0.08)	2(2, 0) - 1(1, 1)	1ν ₄₂	[68046]
	20562.78	(0.08)	2(2, 0) - 1(1, 1)		[68046]
	21252.57	(0.08)	3(1, 2) - 2(2, 1)		[68046]
	21258.43	(0.08)	3(1, 2) - 2(2, 1)	1ν ₄₂	[68046]
	21886.51	(0.08)	3(2, 2) - 2(1, 1)	1ν ₄₂	[68046]
	21904.66	(0.08)	3(2, 2) - 2(1, 1)		[68046]
	22576.76	(0.10)	4(1, 4) - 3(0, 3)		[69061]
	26350.00	(0.10)	3(3, 1) - 2(2, 0)		[69061]
	26699.18	(0.10)	4(1, 3) - 3(2, 2)		[69061]
26771.22	(0.10)	4(2, 3) - 3(1, 2)		[69061]	
27701.08	(0.10)	5(1, 5) - 4(0, 4)		[69061]	
27701.08	(0.10)	5(0, 5) - 4(1, 4)		[69061]	
CHCHCD ₂ CH ₂ CH ₂ CD ₂	10587.55	(0.08)	2(0, 2) - 1(1, 1)		[68046]
	11629.92	(0.08)	2(1, 2) - 1(0, 1)		[68046]
	15730.46	(0.08)	3(0, 3) - 2(1, 2)		[68046]
	16027.97	(0.08)	3(1, 3) - 2(0, 2)		[68046]
	16148.49	(0.08)	2(2, 1) - 1(1, 0)		[68046]
	17337.47	(0.08)	3(1, 2) - 2(2, 1)		[68046]
CDCDCD ₂ CD ₂ CD ₂ CD ₂	20833.80	(0.08)	3(2, 2) - 2(1, 1)		[68046]
	13243.03	(0.08)	2(2, 1) - 1(1, 0)		[68046]
	13965.86	(0.08)	3(0, 3) - 2(1, 2)		[68046]
	13986.47	(0.08)	3(1, 3) - 2(0, 2)		[68046]
	15965.75	(0.08)	2(2, 0) - 1(1, 1)		[68046]
	17384.97	(0.08)	3(2, 2) - 2(1, 1)		[68046]
	23088.55	(0.08)	3(3, 0) - 2(2, 1)		[68046]
	25809.19	(0.08)	3(2, 1) - 2(1, 2)		[68046]

Table 68.1. Molecular constants of endo- and exo-2-methylbicyclo[2.1.0]pentane.

Parameter	endo - C ₆ H ₁₀ ^a	exo - C ₆ H ₁₀ ^a
A (MHz)	6257.3245(58)	7418.7630(64)
B (MHz)	3412.223(6)	3101.651(3)
C (MHz)	2843.403(13)	2652.5494(25)
μ_a (D)	0.050(11)	0.064(1)
μ_b (D)	0.121(24)	0.038(3)
μ_c (D)	0.264(1)	0.160(1)

^aRotational constants from present work, dipole moment values from [75053].

TABLE 68.2. Microwave spectrum of 2-methylbicyclo[2.1.0]pentane

C₆H₁₀

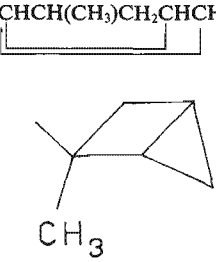
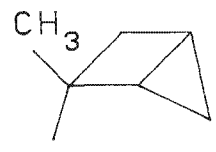
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J''(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
$en\text{-CHCH}(\text{CH}_3)\text{CH}_2\text{CHCH}_2$ 	27923.83	(0.10)	6(5, 2) - 6(4, 2)	[75053]
	28007.20	(0.10)	5(5, 0) - 5(4, 2)	[75053]
	29008.77	(0.10)	3(2, 2) - 2(1, 2)	[75053]
	31145.06	(0.10)	4(1, 3) - 3(0, 3)	[75053]
	32696.11	(0.10)	4(2, 3) - 3(1, 2)	[75053]
	33770.32	(0.10)	4(2, 2) - 3(1, 2)	[75053]
	34382.78	(0.10)	3(3, 1) - 2(2, 0)	[75053]
	34389.37	(0.10)	3(3, 0) - 2(2, 0)	[75053]
	34459.83	(0.10)	3(3, 1) - 2(2, 1)	[75053]
	34466.46	(0.10)	3(3, 0) - 2(2, 1)	[75053]
	36102.56	(0.10)	4(2, 3) - 3(1, 3)	[75053]
	37176.78	(0.10)	4(2, 2) - 3(1, 3)	[75053]
	39917.06	(0.10)	12(7, 6) - 12(6, 6)	[75053]
	39949.15	(0.10)	12(7, 5) - 12(6, 7)	[75053]
$ex\text{-CHCH}(\text{CH}_3)\text{CH}_2\text{CHCH}_2$ 	29876.11	(0.10)	4(1, 3) - 3(0, 3)	[75053]
	30219.19	(0.10)	5(1, 5) - 4(0, 4)	[75053]
	30379.03	(0.10)	3(2, 1) - 2(1, 1)	[75053]
	31561.28	(0.10)	3(2, 2) - 2(1, 2)	[75053]
	32951.87	(0.10)	6(1, 6) - 5(1, 5)	[75053]
	33520.42	(0.10)	6(0, 6) - 5(0, 5)	[75053]
	35016.19	(0.10)	6(1, 6) - 5(0, 5)	[75053]
	35777.23	(0.10)	4(2, 2) - 3(1, 2)	[75053]
	36912.78	(0.10)	5(1, 4) - 4(0, 4)	[75053]
	37983.32	(0.10)	4(2, 3) - 3(1, 3)	[75053]
	39959.22	(0.10)	3(3, 0) - 2(2, 0)	[75053]
	39990.92	(0.10)	3(3, 1) - 2(2, 1)	[75053]

Table 69.1. Molecular constants of methylenecyclopentane.

State ^a	A (MHz)	B (MHz)	C (MHz)	Reference
(0,0)	6493.987(10)	3255.3888(22)	2350.2212(20)	[present]
(0,1)	6466.75(10)	3261.01(1)	2356.10(1)	[72068]
(0,2)	6439.37(8)	3266.62(1)	2362.16(1)	[72068]
(0,3)	6412.05(6)	3272.18(1)	2368.31(1)	[72068]
(0,4)	6385.25(7)	3277.54(1)	2374.41(1)	[72068]
(0,5)	6359.22(6)	3282.61(1)	2380.30(1)	[72068]
(1,0)	6482.43(11)	3253.09(1)	2346.37(1)	[72068]
<u>Electric Dipole Moment</u> [72068]				
μ_a (D)	0.60(1)			
μ_c (D)	0.00(6)			

^aThe lowest energy vibrational mode is a ring bending mode and is designated ν_{42} . The next lowest energy mode is a ring twist and is designated ν_{41} . The state designation is (ν_{41}, ν_{42}) , where the number designates the number of vibrational quanta present in each mode.

TABLE 69.2. Microwave spectrum of methylenecyclopentane

C₆H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
C(CH ₂)CH ₂ CH ₂ CH ₂ CH ₂	18060.55	(0.03)	3(1, 2) - 2(1, 1)		[72068]
	20332.31	(0.03)	4(1, 4) - 3(1, 3)		[72068]
	21025.53	(0.03)	4(0, 4) - 3(0, 3)		[72068]
H ₂ C=C=CH ₂	21761.67	(0.03)	9(2, 7) - 9(2, 8)		[72068]
	22293.33	(0.03)	4(2, 3) - 3(2, 2)		[72068]
H ₂ C CH ₂	22702.16	(0.03)	4(3, 2) - 3(3, 1)		[72068]
	22814.13	(0.03)	4(3, 1) - 3(3, 0)		[72068]
\ / CH ₂	23688.46	(0.03)	4(2, 2) - 3(2, 1)		[72068]
	23841.07	(0.03)	4(1, 3) - 3(1, 2)		[72068]
	25213.60	(0.03)	5(1, 5) - 4(1, 4)		[72068]
	25676.60	(0.03)	5(0, 5) - 4(0, 4)		[72068]
	26079.84	(0.03)	8(3, 6) - 8(1, 7)		[72068]
	20376.86	(0.03)	4(1, 4) - 3(1, 3)	1ν ₄₂	[72068]
	21063.27	(0.03)	4(0, 4) - 3(0, 3)	1ν ₄₂	[72068]
	22338.20	(0.03)	4(2, 3) - 3(2, 2)	1ν ₄₂	[72068]
	23741.53	(0.03)	4(2, 2) - 3(2, 1)	1ν ₄₂	[72068]
	23882.66	(0.03)	4(1, 3) - 3(1, 2)	1ν ₄₂	[72068]
	25268.43	(0.03)	5(1, 5) - 4(1, 4)	1ν ₄₂	[72068]
	25724.28	(0.03)	5(0, 5) - 4(0, 4)	1ν ₄₂	[72068]
	20422.62	(0.03)	4(1, 4) - 3(1, 3)	2ν ₄₂	[72068]
	21102.08	(0.03)	4(0, 4) - 3(0, 3)	2ν ₄₂	[72068]
	22383.87	(0.03)	4(2, 3) - 3(2, 2)	2ν ₄₂	[72068]
	23795.01	(0.03)	4(2, 2) - 3(2, 1)	2ν ₄₂	[72068]
	23924.76	(0.03)	4(1, 3) - 3(1, 2)	2ν ₄₂	[72068]
	25324.70	(0.03)	5(1, 5) - 4(1, 4)	2ν ₄₂	[72068]
	25773.47	(0.03)	5(0, 5) - 4(0, 4)	2ν ₄₂	[72068]
	20468.81	(0.03)	4(1, 4) - 3(1, 3)	3ν ₄₂	[72068]
	21141.36	(0.03)	4(0, 4) - 3(0, 3)	3ν ₄₂	[72068]
	22429.65	(0.03)	4(2, 3) - 3(2, 2)	3ν ₄₂	[72068]
	23848.29	(0.03)	4(2, 2) - 3(2, 1)	3ν ₄₂	[72068]
	23966.69	(0.03)	4(1, 3) - 3(1, 2)	3ν ₄₂	[72068]
	25381.61	(0.03)	5(1, 5) - 4(1, 4)	3ν ₄₂	[72068]
	25823.37	(0.03)	5(0, 5) - 4(0, 4)	3ν ₄₂	[72068]
	20514.40	(0.03)	4(1, 4) - 3(1, 3)	4ν ₄₂	[72068]
	21180.11	(0.03)	4(0, 4) - 3(0, 3)	4ν ₄₂	[72068]
	22474.53	(0.03)	4(2, 3) - 3(2, 2)	4ν ₄₂	[72068]
	23900.16	(0.03)	4(2, 2) - 3(2, 1)	4ν ₄₂	[72068]
	24007.54	(0.03)	4(1, 3) - 3(1, 2)	4ν ₄₂	[72068]
	25437.86	(0.03)	5(1, 5) - 4(1, 4)	4ν ₄₂	[72068]
	25872.76	(0.03)	5(0, 5) - 4(0, 4)	4ν ₄₂	[72068]
	20558.27	(0.03)	4(1, 4) - 3(1, 3)	5ν ₄₂	[72068]
	22517.43	(0.03)	4(2, 3) - 3(2, 2)	5ν ₄₂	[72068]
	24046.34	(0.03)	4(1, 3) - 3(1, 2)	5ν ₄₂	[72068]
	25491.99	(0.03)	5(1, 5) - 4(1, 4)	5ν ₄₂	[72068]
	25920.33	(0.03)	5(0, 5) - 4(0, 4)	5ν ₄₂	[72068]
	20303.15	(0.03)	4(1, 4) - 3(1, 3)	1ν ₄₁	[72068]
	23669.45	(0.03)	4(2, 2) - 3(2, 1)	1ν ₄₁	[72068]
	23817.02	(0.03)	4(1, 3) - 3(1, 2)	1ν ₄₁	[72068]
	25176.40	(0.03)	5(1, 5) - 4(1, 4)	1ν ₄₁	[72068]
	25636.90	(0.03)	5(0, 5) - 4(0, 4)	1ν ₄₁	[72068]

Table 70.1. Molecular constants of bicyclo[3.1.0]hexane.

Parameter	Value
<u>Rotational Constants</u> [present]	
A (MHz)	5542.955(7)
B (MHz)	4236.8179(35)
C (MHz)	3127.0400(33)
<u>Electric Dipole Moment</u> [74065]	
μ_a (D)	0.093(1)
μ_c (D)	0.168(2)

TABLE 70.2. Microwave spectrum of bicyclo[3.1.0]hexane

C₆H₁₀

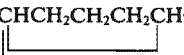
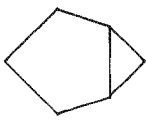
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
CHCH ₂ CH ₂ CH ₂ CHCH ₂ 	26577.31	(0.05)	4(1, 4) - 3(1, 3)	[74065]
	26748.10	(0.05)	4(0, 4) - 3(0, 3)	[74065]
	27362.41	(0.05)	3(1, 2) - 2(0, 2)	[74065]
	27973.74	(0.05)	3(2, 1) - 2(1, 1)	[74065]
	29075.87	(0.05)	4(2, 3) - 3(2, 2)	[74065]
	29339.37	(0.05)	3(2, 2) - 2(1, 2)	[74065]
	30114.15	(0.05)	4(3, 2) - 3(3, 1)	[74065]
	30312.35	(0.05)	4(1, 3) - 3(1, 2)	[74065]
	31316.32	(0.05)	3(3, 0) - 2(2, 0)	[74065]
	31646.75	(0.05)	3(3, 1) - 2(2, 1)	[74065]
	31750.60	(0.05)	4(2, 2) - 3(2, 1)	[74065]
	32886.70	(0.05)	5(1, 5) - 4(1, 4)	[74065]
	32940.86	(0.05)	5(0, 5) - 4(0, 4)	[74065]
	35797.67	(0.05)	5(2, 4) - 4(2, 3)	[74065]
	36354.53	(0.05)	4(2, 2) - 3(1, 2)	[74065]
	36619.53	(0.05)	5(1, 4) - 4(1, 3)	[74065]
	37079.70	(0.05)	4(1, 3) - 3(0, 3)	[74065]
	37504.15	(0.05)	5(3, 3) - 4(3, 2)	[74065]
	37840.80	(0.05)	5(4, 2) - 4(4, 1)	[74065]
	38078.61	(0.05)	5(4, 1) - 4(4, 0)	[74065]
	38238.34	(0.05)	4(2, 3) - 3(1, 3)	[74065]
	38546.16	(0.05)	4(3, 1) - 3(2, 1)	[74065]

Table 71.1. Molecular constants for 1,3,5-heptatriyne (CH₃C₆H). [78034]

Parameter	Ground State	$\nu_{18} = 1$	$\nu_{17} = 1$
B ₀ (MHz)	778.2445(5)	779.5329(6)	779.2686(6)
D _J (kHz)	0.0092(5)	0.0092(5)	0.0072(8)
D _{JK} (kHz)	4.442(4)	4.455(5)	4.472(9)
η_J (kHz)	---	8.14(1)	9.48(3)
q ₁ (kHz)	---	568.0(20)	225.0(30)
ρ	---	0.9836(2)	0.9717(7)

TABLE 71.2. Microwave spectrum of 1,3,5-heptatriyne

C₇H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	J' (K) - J'' (K)	Vib. state	Ref.
CH ₃ (CC) ₃ H	28010.88	(0.03)	18(6) - 17(6)		[78034]
	28012.58	(0.03)	18(5) - 17(5)		[78034]
	28014.02	(0.03)	18(4) - 17(4)		[78034]
	28015.15	(0.03)	18(3) - 17(3)		[78034]
	28015.92	(0.03)	18(2) - 17(2)		[78034]
	28016.45	(0.03)	18(1) - 17(1)		[78034]
	28016.57	(0.03)	18(0) - 17(0)		[78034]
	29566.97	(0.03)	19(6) - 18(6)		[78034]
	29568.82	(0.03)	19(5) - 18(5)		[78034]
	29570.29	(0.03)	19(4) - 18(4)		[78034]
	29571.47	(0.03)	19(3) - 18(3)		[78034]
	29572.39	(0.03)	19(2) - 18(2)		[78034]
	29572.96	(0.03)	19(1) - 18(1)		[78034]
	29573.02	(0.03)	19(0) - 18(0)		[78034]
	31123.10	(0.03)	20(6) - 19(6)		[78034]
	31125.05	(0.03)	20(5) - 19(5)		[78034]
	31126.62	(0.03)	20(4) - 19(4)		[78034]
	31127.88	(0.03)	20(3) - 19(3)		[78034]
	31128.72	(0.03)	20(2) - 19(2)		[78034]
	31129.30	(0.03)	20(1) - 19(1)		[78034]
	31129.47	(0.03)	20(0) - 19(0)		[78034]
	32676.82	(0.03)	21(7) - 20(7)		[78034]
	32679.20	(0.03)	21(6) - 20(6)		[78034]
	32681.28	(0.03)	21(5) - 20(5)		[78034]
	32682.95	(0.03)	21(4) - 20(4)		[78034]
	32684.25	(0.03)	21(3) - 20(3)		[78034]
	32685.20	(0.03)	21(2) - 20(2)		[78034]
	32685.78	(0.03)	21(1) - 20(1)		[78034]
	32685.91	(0.03)	21(0) - 20(0)		[78034]
	34232.79	(0.03)	22(7) - 21(7)		[78034]
	34235.33	(0.03)	22(6) - 21(6)		[78034]
	34237.48	(0.03)	22(5) - 21(5)		[78034]
	34239.25	(0.03)	22(4) - 21(4)		[78034]
	34240.61	(0.03)	22(3) - 21(3)		[78034]
	34241.57	(0.03)	22(2) - 21(2)		[78034]
	34242.20	(0.03)	22(1) - 21(1)		[78034]
	34242.35	(0.03)	22(0) - 21(0)		[78034]
	35782.20	(0.03)	23(9) - 22(9)		[78034]
	35785.72	(0.03)	23(8) - 22(8)		[78034]
	35788.81	(0.03)	23(7) - 22(7)		[78034]
	35791.42	(0.03)	23(6) - 22(6)		[78034]
	35793.71	(0.03)	23(5) - 22(5)		[78034]
	35795.55	(0.03)	23(4) - 22(4)		[78034]
	35796.95	(0.03)	23(3) - 22(3)		[78034]
	35797.98	(0.03)	23(2) - 22(2)		[78034]
	35798.62	(0.03)	23(1) - 22(1)		[78034]
	35798.79	(0.03)	23(0) - 22(0)		[78034]
	37337.95	(0.03)	24(9) - 23(9)		[78034]
	37341.62	(0.03)	24(8) - 23(8)		[78034]
	37344.77	(0.03)	24(7) - 23(7)		[78034]
	37347.55	(0.03)	24(6) - 23(6)		[78034]
	37349.91	(0.03)	24(5) - 23(5)		[78034]
	37351.84	(0.03)	24(4) - 23(4)		[78034]
	37353.30	(0.03)	24(3) - 23(3)		[78034]
37354.40	(0.03)	24(2) - 23(2)		[78034]	
37355.00	(0.03)	24(1) - 23(1)		[78034]	
37355.22	(0.03)	24(0) - 23(0)		[78034]	
38903.65	(0.03)	25(6) - 24(6)		[78034]	
38906.09	(0.03)	25(5) - 24(5)		[78034]	
38908.09	(0.03)	25(4) - 24(4)		[78034]	
38909.65	(0.03)	25(3) - 24(3)		[78034]	
38910.75	(0.03)	25(2) - 24(2)		[78034]	
38911.42	(0.03)	25(1) - 24(1)		[78034]	
38911.64	(0.03)	25(0) - 24(0)		[78034]	
38955.05	(0.05)	25(5) - 24(5)	$1\nu_{17} \quad \ell = -1$	[78034]	
38955.28	(0.05)	25(7) - 24(7)	$1\nu_{17} \quad \ell = +1$	[78034]	
38957.47	(0.05)	25(1) - 24(1)	$1\nu_{17} \quad \ell = +1$	[78034]	
38957.48	(0.05)	25(4) - 24(4)	$1\nu_{17} \quad \ell = -1$	[78034]	

TABLE 71.2. Microwave spectrum of 1,3,5-heptatriyne — Continued

C₇H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K) - J''(K)$	Vib. state	Ref.
	38957.88	(0.05)	25(6) - 24(6)	1v ₁₇ $\ell = +1$	[78034]
	38957.90	(0.05)	25(10) - 24(10)	1v ₁₈ $\ell = +1$	[78034]
	38958.50	(0.05)	25(8) - 24(8)	1v ₁₈ $\ell = -1$	[78034]
	38959.57	(0.05)	25(3) - 24(3)	1v ₁₇ $\ell = -1$	[78034]
	38959.69	(0.05)	25(4) - 24(4)	1v ₁₇ $\ell = +1$	[78034]
	38961.15	(0.05)	25(2) - 24(2)	1v ₁₇ $\ell = -1$	[78034]
	38961.23	(0.05)	25(4) - 24(4)	1v ₁₇ $\ell = +1$	[78034]
	38962.31	(0.05)	25(1) - 24(1)	1v ₁₇ $\ell = -1$	[78034]
	38962.31	(0.05)	25(3) - 24(3)	1v ₁₇ $\ell = +1$	[78034]
	38962.34	(0.05)	25(1) - 24(1)	1v ₁₈ $\ell = +1$	[78034]
	38962.91	(0.05)	25(0) - 24(0)	1v ₁₇ $\ell = +1$	[78034]
	38963.03	(0.05)	25(2) - 24(2)	1v ₁₇ $\ell = +1$	[78034]
	38965.23	(0.05)	25(8) - 24(8)	1v ₁₈ $\ell = +1$	[78034]
	38965.50	(0.05)	25(6) - 24(6)	1v ₁₈ $\ell = -1$	[78034]
	38968.20	(0.05)	25(7) - 24(7)	1v ₁₈ $\ell = +1$	[78034]
	38968.33	(0.05)	25(5) - 24(5)	1v ₁₈ $\ell = -1$	[78034]
	38968.98	(0.05)	25(1) - 24(1)	1v ₁₇ $\ell = +1$	[78034]
	38970.71	(0.05)	25(4) - 24(4)	1v ₁₈ $\ell = -1$	[78034]
	38970.71	(0.05)	25(6) - 24(6)	1v ₁₈ $\ell = +1$	[78034]
	38972.72	(0.05)	25(3) - 24(3)	1v ₁₈ $\ell = -1$	[78034]
	38972.72	(0.05)	25(5) - 24(5)	1v ₁₈ $\ell = +1$	[78034]
	38974.17	(0.05)	25(2) - 24(2)	1v ₁₈ $\ell = -1$	[78034]
	38974.40	(0.05)	25(4) - 24(4)	1v ₁₈ $\ell = +1$	[78034]
	38975.13	(0.05)	25(1) - 24(1)	1v ₁₈ $\ell = -1$	[78034]
	38975.43	(0.05)	25(0) - 24(0)	1v ₁₈ $\ell = +1$	[78034]
	38975.64	(0.05)	25(3) - 24(3)	1v ₁₈ $\ell = +1$	[78034]
	38976.73	(0.05)	25(2) - 24(2)	1v ₁₈ $\ell = +1$	[78034]
	38990.26	(0.05)	25(1) - 24(1)	1v ₁₈ $\ell = +1$	[78034]

Table 72.1. Molecular constants of 1,3,5-cycloheptatriene.

Parameter	Value
<u>Rotational Constants</u> [present]	
A'' (MHz)	3697.1399(3186)
B'' (MHz)	3671.0757(3135)
C'' (MHz)	2032.3077(44)
τ_1 (kHz)	-28.727(6485)
τ_2 (kHz)	-6.3714(14052)
τ_3^a (kHz)	9.92(230)
τ_{aaaa} (kHz)	0 ^b
τ_{bbbb} (kHz)	12.59(447)
τ_{cccc} (kHz)	-0.645(200)
<u>Electric Dipole Moment</u> [65033]	
μ_a (D)	0.24(4)
μ_c (D)	0.060(2)

^aValue fixed by setting $R_6 = 0$.^bFixed at zero.

TABLE 72.2. Microwave spectrum of 1,3,5-cycloheptatriene

C₇H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
CHCHCHCHCHCH ₂	21472.60	(0.07)	7(1, 6) - 7(1, 7)	[65033]
	21974.75	(0.07)	5(0, 5) - 4(0, 4)	[65033]
	24761.70	(0.07)	20(13, 7) - 20(13, 8)	[65033]
	24764.00	(0.07)	19(12, 7) - 19(12, 8)	[65033]
	24766.00	(0.07)	18(11, 7) - 18(11, 8)	[65033]
	24767.85	(0.07)	17(10, 7) - 17(10, 8)	[65033]
	24769.35	(0.07)	16(9, 7) - 16(9, 8)	[65033]
	24770.65	(0.07)	15(8, 7) - 15(8, 8)	[65033]
	24771.85	(0.07)	14(7, 7) - 14(7, 8)	[65033]
	24772.90	(0.07)	13(6, 7) - 13(6, 8)	[65033]
	24773.75	(0.07)	12(5, 7) - 12(5, 8)	[65033]
	24774.45	(0.07)	11(4, 7) - 11(4, 8)	[65033]
	24775.10	(0.07)	10(3, 7) - 10(3, 8)	[65033]
	24775.65	(0.07)	9(2, 7) - 9(2, 8)	[65033]
	25278.20	(0.07)	5(1, 4) - 4(1, 3)	[65033]
	26039.20	(0.07)	6(0, 6) - 5(0, 5)	[65033]
	28580.12	(0.07)	5(3, 3) - 4(3, 2)	[65033]
	28584.00	(0.07)	5(2, 3) - 4(2, 2)	[65033]
	34168.23	(0.07)	8(0, 8) - 7(0, 7)	[65033]
	34686.50	(0.07)	11(1, 10) - 11(1, 11)	[65033]

Table 73.1. Molecular constants for toluene.

Species	A (MHz)	B (MHz)	C (MHz)	Reference
Normal	5729.325(217)	2517.447(9)	1748.872(20)	[67039]
Me- ¹³ C	5729.49(15)	2444.590(10)	1713.364(10)	[73085]
1- ¹³ C	5730.215(141)	2506.420(6)	1743.528(6)	[81048]
2- ¹³ C	5638.549(277)	2516.859(16)	1739.904(15)	[81048]
3- ¹³ C	5638.572(100)	2500.599(4)	1732.217(43)	[81048]
4- ¹³ C	5729.63(12)	2474.926(5)	1728.233(5)	[81048]
2-d ₁	5448.87(10)	2509.758(10)	1718.212(10)	[73085]
3-d ₁	5453.73(20)	2480.551(10)	1704.917(10)	[73085]
4-d ₁	5729.56(15)	2413.638(10)	1698.125(10)	[73085]
Me-d ₃	5728.92(20)	2235.981(10)	1608.126(10)	[73085]
<u>Electric Dipole Moment</u> [67034]				
μ_a	0.375(10) D			
<u>Internal Rotation Constants</u> [67034]				
V_6	4.879(35) cm ⁻¹			
I_α	3.14 u Å ² (assumed)			

TABLE 73.2. Microwave spectrum of toluene

C₇H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$	$- J''(K_{-1}, K_{+1})$	V_i	Sym.	Ref.	
CH ₃ CCHCHCHCHCH	8410.480	(0.100)	2(0, 2)	- 1(0, 1)	0		[67034]	
	9301.265	(0.100)	2(1, 1)	- 1(1, 0)	0		[67034]	
	11574.972	(0.100)	3(1, 3)	- 2(1, 2)	0		[67034]	
	11955.096	(0.100)	3(1, 0)	- 2(1, 0)	3	--	[67034]	
	12013.284	(0.100)	3(1, 0)	- 2(1, 0)	3	++	[67034]	
	12329.477	(0.100)	3(0, 3)	- 2(0, 2)	0		[67034]	
	12798.959	(0.100)	3(2, 2)	- 2(2, 1)	0		[67034]	
	13268.439	(0.100)	3(2, 1)	- 2(2, 0)	0		[67034]	
	13632.894	(0.100)	3(1, 0)	- 2(1, 0)	3	+-	[67034]	
	13685.191	(0.100)	3(1, 0)	- 2(1, 0)	3	-+	[67034]	
	13868.346	(0.100)	3(1, 2)	- 2(1, 1)	0		[67034]	
	15316.424	(0.100)	4(1, 4)	- 3(1, 3)	0		[67034]	
	15993.342	(0.100)	4(0, 4)	- 3(0, 3)	0		[67034]	
	16969.560	(0.100)	4(2, 3)	- 3(2, 2)	0		[67034]	
	17276.662	(0.100)	4(3, 2)	- 3(3, 1)	0		[67034]	
	17349.558	(0.100)	4(3, 1)	- 3(3, 0)	0		[67034]	
	18040.710	(0.100)	4(2, 2)	- 3(2, 1)	0		[67034]	
	18987.870	(0.100)	5(1, 5)	- 4(1, 4)	0		[67034]	
	19479.420	(0.100)	5(0, 5)	- 4(0, 4)	0		[67034]	
	21610.498	(0.100)	5(4, 1)	- 4(4, 0)	0		[67034]	
	21638.614	(0.100)	5(3, 3)	- 4(3, 2)	0		[67034]	
	21883.133	(0.100)	5(3, 2)	- 4(3, 1)	0		[67034]	
	22902.321	(0.100)	6(0, 6)	- 5(0, 5)	0		[67034]	
	22905.278	(0.100)	5(2, 3)	- 4(2, 2)	0		[67034]	
	¹³ CH ₃ CCHCHCHCHCH	8206.913	(0.100)	2(0, 2)	- 1(0, 1)	0		[73085]
		9047.110	(0.100)	2(1, 1)	- 1(1, 0)	0		[73085]
		11313.306	(0.100)	3(1, 3)	- 2(1, 2)	0		[73085]
		11669.844	(0.100)	3(1, 0)	- 2(1, 0)	3		[73085]
		11723.760	(0.100)	3(1, 0)	- 2(1, 0)	3		[73085]
		12052.883	(0.100)	3(0, 3)	- 2(0, 2)	0		[73085]
12473.832		(0.100)	3(2, 2)	- 2(2, 1)	0		[73085]	
12894.873		(0.100)	3(2, 1)	- 2(2, 0)	0		[73085]	
13268.635		(0.100)	3(1, 0)	- 2(1, 0)	3		[73085]	
13317.131		(0.100)	3(1, 0)	- 2(1, 0)	3		[73085]	
13496.681		(0.100)	3(1, 2)	- 2(1, 1)	0		[73085]	
14978.760		(0.100)	4(1, 4)	- 3(1, 3)	0		[73085]	
15541.200		(0.100)	4(1, 0)	- 3(1, 0)	3		[73085]	
15747.808		(0.100)	4(1, 0)	- 3(1, 0)	3		[73085]	
16546.547		(0.100)	4(2, 3)	- 3(2, 2)	0		[73085]	
16822.389		(0.100)	4(3, 2)	- 3(3, 1)	0		[73085]	
16883.249		(0.100)	4(3, 1)	- 3(3, 0)	0		[73085]	
17668.095		(0.100)	4(1, 0)	- 3(1, 0)	3		[73085]	
17841.894		(0.100)	4(1, 0)	- 3(1, 0)	3		[73085]	
17842.803		(0.100)	4(1, 3)	- 3(1, 2)	0		[73085]	
18579.170		(0.100)	5(1, 5)	- 4(1, 4)	0		[73085]	
20547.911		(0.100)	5(2, 4)	- 4(2, 3)	0		[73085]	
21031.546		(0.100)	5(4, 2)	- 4(4, 1)	0		[73085]	
21037.882		(0.100)	5(4, 1)	- 4(4, 0)	0		[73085]	
21069.089		(0.100)	5(3, 3)	- 4(3, 2)	0		[73085]	
21275.174		(0.100)	5(3, 2)	- 4(3, 1)	0		[73085]	
22028.978		(0.100)	5(1, 4)	- 4(1, 3)	0		[73085]	
22121.898		(0.100)	6(1, 6)	- 5(1, 5)	0		[73085]	
22237.933		(0.100)	5(2, 3)	- 4(2, 2)	0		[73085]	
22452.914		(0.100)	6(0, 6)	- 5(0, 5)	0		[73085]	
CH ₃ ¹³ CCHCHCHCHCH	17961.0	(0.1)	4(2, 2)	- 3(2, 1)	0		[81048]	
	18246.53	(0.10)	4(1, 3)	- 3(1, 2)	0		[81048]	
	18926.20	(0.10)	5(1, 4)	- 4(1, 4)	0		[81048]	
	19421.45	(0.10)	5(0, 5)	- 4(0, 4)	0		[81048]	
	20983.51	(0.10)	5(2, 4)	- 4(2, 3)	0		[81048]	
	21552.38	(0.10)	5(3, 3)	- 4(3, 2)	0		[81048]	
	21791.06	(0.10)	5(3, 2)	- 4(3, 1)	0		[81048]	
	22501.92	(0.10)	5(1, 4)	- 4(1, 3)	0		[81048]	
	22526.68	(0.10)	6(1, 6)	- 5(1, 5)	0		[81048]	
	22804.09	(0.10)	5(2, 3)	- 4(2, 2)	0		[81048]	
	22835.12	(0.10)	6(0, 6)	- 5(0, 5)	0		[81048]	
	24968.49	(0.10)	6(2, 5)	- 5(2, 4)	0		[81048]	
	25880.78	(0.10)	6(3, 4)	- 5(3, 3)	0		[81048]	
	25897.28	(0.10)	6(4, 3)	- 5(4, 2)	0		[81048]	

TABLE 73.2. Microwave spectrum of toluene — Continued

C₇H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	V_i	Sym.	Ref.
	25931.89	(0.10)	6(4, 2) - 5(4, 1)	0		[81048]
	26254.19	(0.10)	7(0, 7) - 6(0, 6)	0		[81048]
	28853.25	(0.10)	7(2, 6) - 6(2, 5)	0		[81048]
	30089.67	(0.10)	7(6, 2) - 6(6, 1)	0		[81048]
	30164.25	(0.10)	7(3, 5) - 6(3, 4)	0		[81048]
	30179.51	(0.10)	7(5, 3) - 6(5, 2)	0		[81048]
	30183.27	(0.10)	7(5, 2) - 6(5, 1)	0		[81048]
	30417.63	(0.10)	7(4, 3) - 6(4, 2)	0		[81048]
	32237.10	(0.10)	7(2, 5) - 6(2, 4)	0		[81048]
	32638.30	(0.10)	8(2, 7) - 7(2, 6)	0		[81048]
	34588.86	(0.10)	8(5, 4) - 7(5, 3)	0		[81048]
	34729.20	(0.10)	8(4, 5) - 7(4, 4)	0		[81048]
	35019.83	(0.10)	8(4, 4) - 7(4, 3)	0		[81048]
	36333.78	(0.10)	9(2, 8) - 8(2, 7)	0		[81048]
	36650.34	(0.10)	8(2, 6) - 7(2, 5)	0		[81048]
	39031.15	(0.10)	9(5, 5) - 8(5, 4)	0		[81048]
	39080.35	(0.10)	9(5, 4) - 8(5, 3)	0		[81048]
	39144.06	(0.10)	9(4, 6) - 8(4, 5)	0		[81048]
	39784.57	(0.10)	9(4, 5) - 8(4, 4)	0		[81048]
CH ₃ CCH ¹³ CHCHCH	28846.58	(0.10)	7(2, 6) - 7(2, 5)	0		[81048]
	30159.70	(0.10)	7(6, 1) - 6(6, 0)	0		[81048]
	30218.70	(0.10)	7(3, 5) - 6(3, 4)	0		[81048]
	30255.26	(0.10)	7(5, 3) - 6(5, 2)	0		[81048]
	30260.03	(0.10)	7(6, 1) - 6(6, 0)	0		[81048]
	30385.97	(0.10)	7(4, 4) - 6(4, 3)	0		[81048]
	32323.80	(0.10)	7(2, 5) - 6(2, 4)	0		[81048]
	32614.27	(0.10)	8(2, 7) - 7(2, 6)	0		[81048]
	34420.80	(0.10)	8(3, 6) - 7(3, 5)	0		[81048]
	34456.52	(0.10)	8(7, 2) - 7(7, 1)	0		[81048]
	34820.93	(0.10)	8(4, 5) - 7(4, 4)	0		[81048]
	35155.62	(0.10)	8(4, 4) - 7(4, 3)	0		[81048]
	36539.32	(0.10)	8(3, 5) - 7(3, 4)	0		[81048]
	38519.32	(0.10)	9(3, 7) - 8(3, 6)	0		[81048]
	38832.75	(0.10)	9(7, 3) - 8(7, 2)	0		[81048]
	38955.00	(0.10)	9(6, 4) - 8(6, 3)	0		[81048]
	38957.23	(0.10)	9(6, 3) - 8(6, 2)	0		[81048]
	39141.45	(0.10)	9(5, 5) - 8(5, 4)	0		[81048]
	39200.82	(0.10)	9(5, 4) - 8(5, 3)	0		[81048]
CH ₃ CCHCH ¹³ CHCH	15842.80	(0.10)	4(0, 4) - 3(0, 3)	0		[81048]
	18177.00	(0.10)	4(1, 3) - 3(1, 2)	0		[81048]
	22679.60	(0.10)	6(0, 6) - 5(0, 5)	0		[81048]
	22753.15	(0.10)	5(2, 3) - 4(2, 2)	0		[81048]
	25785.44	(0.10)	6(3, 4) - 5(3, 3)	0		[81048]
	26077.63	(0.10)	7(0, 7) - 6(0, 6)	0		[81048]
	26415.20	(0.10)	6(3, 3) - 5(3, 2)	0		[81048]
	29982.90	(0.10)	7(6, 2) - 6(6, 1)	0		[81048]
	30046.80	(0.10)	7(3, 5) - 6(3, 4)	0		[81048]
	30076.05	(0.10)	7(5, 3) - 6(5, 2)	0		[81048]
	30080.51	(0.10)	7(5, 2) - 6(5, 1)	0		[81048]
	30204.76	(0.10)	7(4, 4) - 6(4, 3)	0		[81048]
	30327.41	(0.10)	7(4, 3) - 6(4, 2)	0		[81048]
	31293.70	(0.10)	7(3, 4) - 6(3, 3)	0		[81048]
	32455.75	(0.10)	8(2, 7) - 7(2, 6)	0		[81048]
	32900.21	(0.10)	9(1, 9) - 8(1, 8)	0		[81048]
	34473.94	(0.10)	8(5, 4) - 7(5, 3)	0		[81048]
	34491.55	(0.10)	8(5, 3) - 7(5, 2)	0		[81048]
	36119.90	(0.10)	9(2, 8) - 8(2, 7)	0		[81048]
	36500.10	(0.10)	8(2, 6) - 7(2, 5)	0		[81048]
	38312.50	(0.10)	9(3, 7) - 8(3, 6)	0		[81048]
	38723.30	(0.10)	9(6, 4) - 8(6, 3)	0		[81048]
	38905.60	(0.10)	9(5, 5) - 8(5, 4)	0		[81048]
	38961.20	(0.10)	9(5, 4) - 8(5, 3)	0		[81048]
	39010.40	(0.10)	9(4, 6) - 8(4, 5)	0		[81048]
	39707.29	(0.10)	9(4, 5) - 8(4, 4)	0		[81048]
CH ₃ CCHCH ¹³ CHCH	30939.10	(0.10)	7(3, 4) - 6(3, 3)	0		[81048]
	31858.33	(0.10)	7(2, 5) - 6(2, 4)	0		[81048]
	32234.10	(0.10)	8(2, 7) - 7(2, 6)	0		[81048]

TABLE 73.2. Microwave spectrum of toluene — Continued

C₇H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	V_i	Sym.	Ref.
	32821.08	(0.10)	9(1, 9) - 8(1, 8)	0		[81048]
	32869.53	(0.10)	9(0, 9) - 8(0, 8)	0		[81048]
	33432.34	(0.10)	8(1, 7) - 7(1, 6)	0		[81048]
	33999.10	(0.10)	8(3, 6) - 7(3, 5)	0		[81048]
	34325.30	(0.10)	8(4, 5) - 7(4, 4)	0		[81048]
	34588.50	(0.10)	8(4, 4) - 7(4, 3)	0		[81048]
	35870.50	(0.10)	8(3, 5) - 7(3, 4)	0		[81048]
	35993.78	(0.10)	9(2, 8) - 8(2, 7)	0		[81048]
	36245.65	(0.10)	8(2, 6) - 7(2, 5)	0		[81048]
	38079.67	(0.10)	9(3, 7) - 8(3, 6)	0		[81048]
CH ₃ CCHCDCHCHCH	8316.483	(0.100)	2(0, 2) - 1(0, 1)	0		[73085]
	9247.530	(0.100)	2(1, 1) - 1(1, 0)	0		[73085]
	11415.948	(0.100)	3(1, 3) - 2(1, 2)	0		[73085]
	11782.584	(0.100)	3(1, 0) - 2(1, 0)	3		[73085]
	11854.452	(0.100)	3(1, 0) - 2(1, 0)	3		[73085]
	12152.573	(0.100)	3(0, 3) - 2(0, 2)	0		[73085]
	12683.916	(0.100)	3(2, 2) - 2(2, 1)	0		[73085]
	13215.246	(0.100)	3(2, 1) - 2(2, 0)	0		[73085]
	13569.180	(0.100)	3(1, 0) - 2(1, 0)	3		[73085]
	13633.489	(0.100)	3(1, 0) - 2(1, 0)	3		[73085]
	13774.966	(0.100)	3(1, 2) - 2(1, 1)	0		[73085]
	15090.680	(0.100)	4(1, 4) - 3(1, 3)	0		[73085]
	15684.080	(0.100)	4(1, 0) - 3(1, 0)	3		[73085]
	15718.480	(0.100)	4(0, 4) - 3(0, 3)	0		[73085]
	15953.604	(0.100)	4(1, 0) - 3(1, 0)	3		[73085]
	16802.601	(0.100)	4(2, 2) - 3(2, 2)	0		[73085]
	17150.001	(0.100)	4(3, 2) - 3(3, 1)	0		[73085]
	17241.864	(0.100)	4(3, 1) - 3(3, 0)	0		[73085]
	17994.545	(0.100)	4(2, 2) - 3(2, 1)	0		[73085]
	18059.482	(0.100)	4(1, 0) - 3(1, 0)	3		[73085]
	18164.932	(0.100)	4(1, 3) - 3(1, 2)	0		[73085]
	18282.267	(0.100)	4(1, 0) - 3(1, 0)	3		[73085]
	18690.111	(0.100)	5(1, 5) - 4(1, 4)	0		[73085]
	19118.180	(0.100)	5(0, 5) - 4(0, 4)	0		[73085]
	20830.823	(0.100)	5(2, 4) - 4(2, 3)	0		[73085]
	21448.886	(0.100)	5(4, 2) - 4(4, 1)	0		[73085]
	21460.282	(0.100)	5(4, 1) - 4(4, 0)	0		[73085]
	21478.168	(0.100)	5(3, 3) - 4(3, 2)	0		[73085]
	21784.936	(0.100)	5(3, 2) - 4(3, 1)	0		[73085]
	22227.572	(0.100)	6(1, 6) - 5(1, 5)	0		[73085]
	22340.835	(0.100)	5(1, 4) - 4(1, 3)	0		[73085]
	22476.006	(0.100)	6(0, 6) - 5(0, 5)	0		[73085]
	22841.039	(0.100)	5(2, 3) - 4(2, 2)	0		[73085]
CH ₃ CCDCHCHCHCH	8238.026	(0.100)	2(0, 2) - 1(0, 1)	0		[73085]
	9146.530	(0.100)	2(1, 1) - 1(1, 0)	0		[73085]
	11315.961	(0.100)	3(1, 3) - 2(1, 2)	0		[73085]
	11684.394	(0.100)	3(1, 0) - 2(1, 0)	3		[73085]
	11752.524	(0.100)	3(1, 0) - 2(1, 0)	3		[73085]
	12048.664	(0.100)	3(0, 3) - 2(0, 2)	0		[73085]
	12556.477	(0.100)	3(2, 2) - 2(2, 1)	0		[73085]
	13064.270	(0.100)	3(2, 1) - 2(2, 0)	0		[73085]
	13416.979	(0.100)	3(1, 0) - 2(1, 0)	3		[73085]
	13478.565	(0.100)	3(1, 0) - 2(1, 0)	3		[73085]
	13628.372	(0.100)	3(1, 2) - 2(1, 1)	0		[73085]
	14962.640	(0.100)	4(1, 4) - 3(1, 3)	0		[73085]
	15555.320	(0.100)	4(1, 0) - 3(1, 0)	3		[73085]
	15596.136	(0.100)	4(0, 4) - 3(0, 3)	0		[73085]
	15809.824	(0.100)	4(1, 0) - 3(1, 0)	3		[73085]
	16637.756	(0.100)	4(2, 3) - 3(2, 2)	0		[73085]
	16969.718	(0.100)	4(3, 2) - 3(3, 1)	0		[73085]
	17054.988	(0.100)	4(3, 1) - 3(3, 0)	0		[73085]
	17782.116	(0.100)	4(2, 2) - 3(2, 1)	0		[73085]
	17858.976	(0.100)	4(1, 0) - 3(1, 0)	3		[73085]
	17979.967	(0.100)	4(1, 3) - 3(1, 2)	0		[73085]
	18071.319	(0.100)	4(1, 0) - 3(1, 0)	3		[73085]
	18536.392	(0.100)	5(1, 5) - 4(1, 4)	0		[73085]
	18975.780	(0.100)	5(0, 5) - 4(0, 4)	0		[73085]

TABLE 73.2. Microwave spectrum of toluene — Continued

C₇H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	V_l	Sym.	Ref.
	20632.698	(0.100)	5(2, 4) - 4(2, 3)	0		[73085]
	21221.956	(0.100)	5(4, 2) - 4(4, 1)	0		[73085]
	21232.164	(0.100)	5(4, 1) - 4(4, 0)	0		[73085]
	21253.141	(0.100)	5(3, 3) - 4(3, 2)	0		[73085]
	21538.278	(0.100)	5(3, 2) - 4(3, 1)	0		[73085]
	22049.149	(0.100)	6(1, 6) - 5(1, 5)	0		[73085]
	22128.994	(0.100)	5(1, 4) - 4(1, 3)	0		[73085]
	22308.750	(0.100)	6(0, 6) - 5(0, 5)	0		[73085]
	22573.883	(0.100)	5(2, 3) - 4(2, 2)	0		[73085]
CH ₃ CCHCDCHCHCH	8119.712	(0.100)	2(0, 2) - 1(0, 1)	0		[73085]
	8938.968	(0.100)	2(1, 1) - 1(1, 0)	0		[73085]
	11201.268	(0.100)	3(1, 3) - 2(1, 2)	0		[73085]
	11547.600	(0.100)	3(1, 0) - 2(1, 0)	3		[73085]
	11599.776	(0.100)	3(1, 0) - 2(1, 0)	3		[73085]
	11933.816	(0.100)	3(0, 3) - 2(0, 2)	0		[73085]
	12335.275	(0.100)	3(2, 2) - 2(2, 1)	0		[73085]
	12736.780	(0.100)	3(2, 1) - 2(2, 0)	0		[73085]
	13114.082	(0.100)	3(1, 0) - 2(1, 0)	3		[73085]
	13161.066	(0.100)	3(1, 0) - 2(1, 0)	3		[73085]
	13338.264	(0.100)	3(1, 2) - 2(1, 1)	0		[73085]
	14833.965	(0.100)	4(1, 4) - 3(1, 3)	0		[73085]
	15378.984	(0.100)	4(1, 0) - 3(1, 0)	3		[73085]
	15518.624	(0.100)	4(0, 4) - 3(0, 3)	0		[73085]
	15578.448	(0.100)	4(1, 0) - 3(1, 0)	3		[73085]
	16365.914	(0.100)	4(2, 3) - 3(2, 2)	0		[73085]
	16629.074	(0.100)	4(3, 2) - 3(3, 1)	0		[73085]
	16685.433	(0.100)	4(3, 1) - 3(3, 0)	0		[73085]
	17293.695	(0.100)	4(2, 2) - 3(2, 1)	0		[73085]
	17463.084	(0.100)	4(1, 0) - 3(1, 0)	3		[73085]
	17631.132	(0.100)	4(1, 0) - 3(1, 0)	3		[73085]
	17639.691	(0.100)	4(1, 3) - 3(1, 2)	0		[73085]
	18403.724	(0.100)	5(1, 5) - 4(1, 4)	0		[73085]
	18927.108	(0.100)	5(0, 5) - 4(0, 4)	0		[73085]
	20328.555	(0.100)	5(2, 4) - 4(2, 3)	0		[73085]
	20789.012	(0.100)	5(4, 2) - 4(4, 1)	0		[73085]
	20794.608	(0.100)	5(4, 1) - 4(4, 0)	0		[73085]
	20826.864	(0.100)	5(3, 3) - 4(3, 2)	0		[73085]
	21018.005	(0.100)	5(3, 2) - 4(3, 1)	0		[73085]
	21789.952	(0.100)	5(1, 4) - 4(1, 3)	0		[73085]
	21917.310	(0.100)	6(1, 6) - 5(1, 5)	0		[73085]
	21954.534	(0.100)	5(2, 3) - 4(2, 2)	0		[73085]
	22259.645	(0.100)	6(0, 6) - 5(0, 5)	0		[73085]
CD ₃ CCHCHCHCHCH	10544.933	(0.100)	3(1, 3) - 2(1, 2)	0		[73085]
	10903.791	(0.100)	3(1, 0) - 2(1, 0)	3		[73085]
	10934.085	(0.100)	3(1, 0) - 2(1, 0)	3		[73085]
	11230.728	(0.100)	3(0, 3) - 2(0, 2)	0		[73085]
	11532.312	(0.100)	3(2, 2) - 2(2, 1)	0		[73085]
	11833.932	(0.100)	3(2, 1) - 2(2, 0)	0		[73085]
	12161.764	(0.100)	3(1, 0) - 2(1, 0)	3		[73085]
	12189.194	(0.100)	3(1, 0) - 2(1, 0)	3		[73085]
	12422.479	(0.100)	3(1, 2) - 2(1, 1)	0		[73085]
	13982.528	(0.100)	4(1, 4) - 3(1, 3)	0		[73085]
	14528.970	(0.100)	4(1, 0) - 3(1, 0)	3		[73085]
	14655.330	(0.100)	4(1, 0) - 3(1, 0)	3		[73085]
	14665.230	(0.100)	4(0, 4) - 3(0, 3)	0		[73085]
	15316.128	(0.100)	4(2, 3) - 3(2, 2)	0		[73085]
	15550.160	(0.100)	4(3, 1) - 3(3, 0)	0		[73085]
	16026.959	(0.100)	4(2, 2) - 3(2, 1)	0		[73085]
	16203.088	(0.100)	4(1, 0) - 3(1, 0)	3		[73085]
	16311.990	(0.100)	4(1, 0) - 3(1, 0)	3		[73085]
	16458.334	(0.100)	4(1, 3) - 3(1, 2)	0		[73085]
	17369.412	(0.100)	5(1, 5) - 4(1, 4)	0		[73085]
	17936.106	(0.100)	5(0, 5) - 4(0, 4)	0		[73085]
	19049.100	(0.100)	5(2, 4) - 4(2, 3)	0		[73085]
	19392.060	(0.100)	5(4, 2) - 4(4, 1)	0		[73085]
	19394.900	(0.100)	5(4, 1) - 4(4, 0)	0		[73085]
	19429.160	(0.100)	5(3, 3) - 4(3, 2)	0		[73085]

TABLE 73.2. Microwave spectrum of toluene — Continued

C₇H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	V_r	Sym.	Ref.
	19551.060	(0.100)	5(3, 2) - 4(3, 1)	0		[73085]
	20330.172	(0.100)	5(2, 3) - 4(2, 2)	0		[73085]
	20386.620	(0.100)	5(1, 4) - 4(1, 3)	0		[73085]
	20708.214	(0.100)	6(1, 6) - 5(1, 5)	0		[73085]
	21114.354	(0.100)	6(0, 6) - 5(0, 5)	0		[73085]
	22720.519	(0.100)	6(2, 5) - 5(2, 4)	0		[73085]
	23323.032	(0.100)	6(4, 3) - 5(4, 2)	0		[73085]
	23336.640	(0.100)	6(4, 2) - 5(4, 1)	0		[73085]
	23342.952	(0.100)	6(3, 4) - 5(3, 3)	0		[73085]
	23655.168	(0.100)	6(3, 3) - 5(3, 2)	0		[73085]

Table 74.1. Molecular constants of the ground state of spiro[2.4]hepta-4,6-diene.

Parameter	Value [present]
A'' (MHz)	6102.1458(157)
B'' (MHz)	2454.22468(128)
C'' (MHz)	2028.89179(132)
τ_1 (kHz)	-6.3183(1441)
τ_2 (kHz)	-1.6455(451)
τ_3^a (kHz)	1.5(14)
τ_{aaaa} (kHz)	0 ^b
τ_{bbbb} (kHz)	-0.76152(4128)
τ_{cccc} (kHz)	-0.3815(419)
<u>Electric Dipole Moment</u> [80035]	
μ_a (D)	0.947(3)

^aValue fixed by setting $R_g = 0$.^bFixed at zero.

Table 74.2. Molecular constants of some isotopically substituted species of spiro[2.4]hepta-4,6-diene. [81040]

Species	A (MHz)	B (MHz)	C (MHz)
1- ¹³ C	6052.345(114)	2410.269(5)	2003.061(3)
3- ¹³ C	6102.025(205)	2451.877(8)	2027.310(5)
4- ¹³ C	6003.000(94)	2452.051(5)	2016.335(3)
5- ¹³ C	6063.945(136)	2419.796(8)	2001.166(4)
1-d ₁	5934.441(19)	2387.133(1)	1988.101(1)
4-d ₁	5766.973(71)	2454.162(2)	1990.343(3)
5-d ₁	5977.960(57)	2375.489(2)	1961.592(2)

TABLE 74.3. Microwave spectrum of spiro[2.4]hepta-4,6-diene

C₇H₈

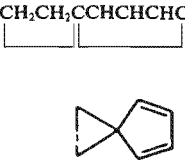
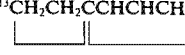
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
$\text{CH}_2\text{CH}_2\text{CCHCHCHCH}$ 	26741.50	(0.05)	6(2, 5) - 5(2, 4)	[81040]
	26986.17	(0.05)	6(5, 1) - 5(5, 0)	[81040]
	26986.17	(0.05)	6(5, 2) - 5(5, 1)	[81040]
	27003.15	(0.05)	12(1,11) - 12(1,12)	[81040]
	27016.76	(0.05)	6(4, 3) - 5(4, 2)	[81040]
	27019.41	(0.05)	6(4, 2) - 5(4, 1)	[81040]
	27044.50	(0.05)	6(3, 4) - 5(3, 3)	[81040]
	27142.94	(0.05)	6(3, 3) - 5(3, 2)	[81040]
	27767.98	(0.05)	6(2, 4) - 5(2, 3)	[81040]
	27795.01	(0.05)	22(4,18) - 22(4,19)	[81040]
	27842.03	(0.05)	6(1, 5) - 5(1, 4)	[81040]
	29533.97	(0.05)	7(1, 7) - 6(1, 6)	[81040]
	29907.30	(0.05)	7(0, 7) - 6(0, 6)	[81040]
	29955.37	(0.05)	13(1,12) - 13(1,13)	[81040]
	30363.26	(0.05)	19(3,16) - 19(3,17)	[81040]
	31058.95	(0.05)	16(2,14) - 16(2,15)	[81040]
	31111.91	(0.05)	7(2, 6) - 6(2, 5)	[81040]
	31479.56	(0.05)	7(6, 1) - 6(6, 0)	[81040]
	31479.56	(0.05)	7(6, 2) - 6(6, 1)	[81040]
	31506.01	(0.05)	7(5, 3) - 6(5, 2)	[81040]
	31506.17	(0.05)	7(5, 2) - 6(5, 1)	[81040]
	31552.44	(0.05)	7(4, 4) - 6(4, 3)	[81040]
	31561.57	(0.05)	7(4, 3) - 6(4, 2)	[81040]
	31571.14	(0.05)	7(3, 5) - 6(3, 4)	[81040]
	31786.10	(0.05)	7(3, 4) - 6(3, 3)	[81040]
	32185.17	(0.05)	23(4,19) - 23(4,20)	[81040]
	32296.06	(0.05)	7(1, 6) - 6(1, 5)	[81040]
	32577.06	(0.05)	7(2, 5) - 6(2, 4)	[81040]
	32822.81	(0.05)	14(1,13) - 14(1,14)	[81040]
	33656.01	(0.05)	8(1, 8) - 7(1, 7)	[81040]
	33923.60	(0.05)	8(0, 8) - 7(0, 7)	[81040]
	34214.11	(0.05)	20(3,17) - 20(3,18)	[81040]
	34335.29	(0.05)	17(2,15) - 17(2,16)	[81040]
	35445.25	(0.05)	8(2, 7) - 7(2, 6)	[81040]
	35622.78	(0.05)	15(1,14) - 15(1,15)	[81040]
	35973.20	(0.05)	8(7, 1) - 7(7, 0)	[81040]
	35973.20	(0.05)	8(7, 2) - 7(7, 1)	[81040]
	35996.69	(0.05)	8(6, 2) - 7(6, 1)	[81040]
	35996.69	(0.05)	8(6, 3) - 7(6, 2)	[81040]
	36090.39	(0.05)	8(3, 6) - 7(3, 5)	[81040]
36100.61	(0.05)	8(4, 5) - 7(4, 4)	[81040]	
36125.51	(0.05)	8(4, 4) - 7(4, 3)	[81040]	
36500.20	(0.05)	8(3, 5) - 7(3, 4)	[81040]	
36501.44	(0.05)	24(4,20) - 24(4,21)	[81040]	
36648.11	(0.05)	8(1, 7) - 7(1, 6)	[81040]	
37361.40	(0.05)	8(2, 6) - 7(2, 5)	[81040]	
37469.99	(0.05)	18(2,16) - 18(2,17)	[81040]	
37758.85	(0.05)	9(1, 9) - 8(1, 8)	[81040]	
37898.60	(0.05)	21(3,18) - 21(3,19)	[81040]	
37939.39	(0.05)	9(0, 9) - 8(0, 8)	[81040]	
38373.20	(0.05)	16(1,15) - 16(1,16)	[81040]	
39739.11	(0.05)	9(2, 8) - 8(2, 7)	[81040]	
$^{13}\text{CH}_2\text{CH}_2\text{CCHCHCHCH}$ 	29515.91	(0.05)	7(0, 7) - 6(0, 6)	[81040]
	29135.08	(0.05)	7(1, 7) - 6(1, 6)	[81040]
	30645.39	(0.05)	7(2, 6) - 6(2, 5)	[81040]
	31070.49	(0.05)	7(3, 5) - 6(3, 4)	[81040]
	31050.18	(0.05)	7(4, 4) - 6(4, 3)	[81040]
	31007.32	(0.05)	7(5, 3) - 6(5, 2)	[81040]
	33205.94	(0.05)	8(1, 8) - 7(1, 7)	[81040]
	34920.80	(0.05)	8(2, 7) - 7(2, 6)	[81040]
	35519.69	(0.05)	8(3, 6) - 7(3, 5)	[81040]
	35523.73	(0.05)	8(4, 5) - 7(4, 4)	[81040]
	37258.07	(0.05)	9(1, 9) - 8(1, 8)	[81040]
	31795.26	(0.05)	7(1, 6) - 6(1, 5)	[81040]
	32014.87	(0.05)	7(2, 5) - 6(2, 4)	[81040]
	31260.58	(0.05)	7(3, 4) - 6(3, 3)	[81040]
	31057.94	(0.05)	7(4, 3) - 6(4, 2)	[81040]
	31007.46	(0.05)	7(5, 2) - 6(5, 1)	[81040]

TABLE 74.3. Microwave spectrum of spiro[2.4]hepta-4,6-diene — Continued

C₇H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.	
CH ₂ CH ₂ ¹³ CCHCHCHCH	33483.85	(0.05)	8(0, 8) - 7(0, 7)	[81040]	
	36722.32	(0.05)	8(2, 6) - 7(2, 5)	[81040]	
	35883.60	(0.05)	8(3, 5) - 7(3, 4)	[81040]	
	35544.74	(0.05)	8(4, 4) - 7(4, 3)	[81040]	
	37448.92	(0.05)	9(0, 9) - 8(0, 8)	[81040]	
	29884.48	(0.05)	7(0, 7) - 6(0, 6)	[81040]	
	29510.49	(0.05)	7(1, 7) - 6(1, 6)	[81040]	
	31085.58	(0.05)	7(2, 6) - 6(2, 5)	[81040]	
	31533.44	(0.05)	7(4, 3) - 6(4, 2)	[81040]	
	31478.28	(0.05)	7(5, 2) - 6(5, 1)	[81040]	
	33897.76	(0.05)	8(0, 8) - 7(0, 7)	[81040]	
	33629.41	(0.05)	8(1, 8) - 7(1, 7)	[81040]	
	35415.61	(0.05)	8(2, 7) - 7(2, 6)	[81040]	
	36068.38	(0.05)	8(4, 5) - 7(4, 4)	[81040]	
	39706.27	(0.05)	9(2, 8) - 8(2, 7)	[81040]	
	32268.56	(0.05)	7(1, 6) - 6(1, 5)	[81040]	
	32546.12	(0.05)	7(2, 5) - 6(2, 4)	[81040]	
	31756.73	(0.05)	7(3, 4) - 6(3, 3)	[81040]	
	31524.35	(0.05)	7(4, 4) - 6(4, 3)	[81040]	
	31478.12	(0.05)	7(5, 3) - 6(5, 2)	[81040]	
	36617.88	(0.05)	8(1, 7) - 7(1, 6)	[81040]	
	37326.34	(0.05)	8(2, 6) - 7(2, 5)	[81040]	
	36092.97	(0.05)	8(4, 4) - 7(4, 3)	[81040]	
	37910.46	(0.05)	9(0, 9) - 8(0, 8)	[81040]	
	CH ₂ CH ₂ C ¹³ CHCHCHCH	29726.90	(0.05)	7(0, 7) - 6(0, 6)	[81040]
		29372.27	(0.05)	7(1, 7) - 6(1, 6)	[81040]
		30989.10	(0.05)	7(2, 6) - 6(2, 5)	[81040]
31477.65		(0.05)	7(3, 5) - 6(3, 4)	[81040]	
31461.79		(0.05)	7(4, 4) - 6(4, 3)	[81040]	
32529.88		(0.05)	7(2, 5) - 6(2, 4)	[81040]	
33466.92		(0.05)	8(1, 8) - 7(1, 7)	[81040]	
35297.15		(0.05)	8(2, 7) - 7(2, 6)	[81040]	
35981.32		(0.05)	8(3, 6) - 7(3, 5)	[81040]	
35999.47		(0.05)	8(4, 5) - 7(4, 4)	[81040]	
37542.35		(0.05)	9(1, 9) - 8(1, 8)	[81040]	
32181.15		(0.05)	7(1, 6) - 6(1, 5)	[81040]	
31718.56		(0.05)	7(3, 4) - 6(3, 3)	[81040]	
31472.64		(0.05)	7(4, 3) - 6(4, 2)	[81040]	
33715.87		(0.05)	8(0, 8) - 7(0, 7)	[81040]	
37298.71		(0.05)	8(2, 6) - 7(2, 5)	[81040]	
36438.15		(0.05)	8(3, 5) - 7(3, 4)	[81040]	
36028.87		(0.05)	8(4, 4) - 7(4, 3)	[81040]	
37706.93		(0.05)	9(0, 9) - 8(0, 8)	[81040]	
CH ₂ CH ₂ CCH ¹³ CHCHCH		29507.17	(0.05)	7(0, 7) - 6(0, 6)	[81040]
		29131.75	(0.05)	7(1, 7) - 6(1, 6)	[81040]
		31337.78	(0.05)	7(3, 4) - 6(3, 3)	[81040]
		31121.08	(0.05)	7(4, 3) - 6(4, 2)	[81040]
		33469.13	(0.05)	8(0, 8) - 7(0, 7)	[81040]
		36834.95	(0.05)	8(2, 6) - 7(2, 5)	[81040]
		35982.09	(0.05)	8(3, 5) - 7(3, 4)	[81040]
		35620.24	(0.05)	8(4, 4) - 7(4, 3)	[81040]
	37429.83	(0.05)	9(0, 9) - 8(0, 8)	[81040]	
	31855.86	(0.05)	7(1, 6) - 6(1, 5)	[81040]	
	30684.73	(0.05)	7(2, 6) - 6(2, 5)	[81040]	
	31131.72	(0.05)	7(3, 5) - 6(3, 4)	[81040]	
	31112.48	(0.05)	7(4, 4) - 6(4, 3)	[81040]	
	33198.44	(0.05)	8(1, 8) - 7(1, 7)	[81040]	
	34960.17	(0.05)	8(2, 7) - 7(2, 6)	[81040]	
	35588.69	(0.05)	8(3, 6) - 7(3, 5)	[81040]	
	35596.72	(0.05)	8(4, 5) - 7(4, 4)	[81040]	
	37246.11	(0.05)	9(1, 9) - 8(1, 8)	[81040]	
	CHDCH ₂ CCHCHCHCH	27148.32	(0.05)	6(1, 5) - 5(1, 4)	[81040]
		29270.19	(0.05)	7(0, 7) - 6(0, 6)	[81040]
		28901.62	(0.05)	7(1, 7) - 6(1, 6)	[81040]
		30381.68	(0.05)	7(2, 6) - 6(2, 5)	[81040]
		30801.03	(0.05)	7(3, 5) - 6(3, 4)	[81040]
		30781.63	(0.05)	7(4, 4) - 6(4, 3)	[81040]

TABLE 74.3. Microwave spectrum of spiro[2.4]hepta-4,6-diene — Continued

C₇H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
	30739.27	(0.05)	7(5, 3) - 6(5, 2)	[81040]
	30715.26	(0.05)	7(6, 2) - 6(6, 1)	[81040]
	35770.26	(0.05)	8(1, 7) - 7(1, 6)	[81040]
	36392.53	(0.05)	8(2, 6) - 7(2, 5)	[81040]
	35573.20	(0.05)	8(3, 5) - 7(3, 4)	[81040]
	35237.38	(0.05)	8(4, 4) - 7(4, 3)	[81040]
	35157.59	(0.05)	8(5, 3) - 7(5, 2)	[81040]
	35121.36	(0.05)	8(6, 2) - 7(6, 1)	[81040]
	35100.06	(0.05)	8(7, 1) - 7(7, 0)	[81040]
	37144.76	(0.05)	9(0, 9) - 8(0, 8)	[81040]
	36961.36	(0.05)	9(1, 9) - 8(1, 8)	[81040]
	39607.74	(0.05)	9(3, 7) - 8(3, 6)	[81040]
	39661.44	(0.05)	9(4, 6) - 8(4, 5)	[81040]
	39585.35	(0.05)	9(5, 5) - 8(5, 4)	[81040]
	39534.75	(0.05)	9(6, 4) - 8(6, 3)	[81040]
	39504.46	(0.05)	9(7, 3) - 8(7, 2)	[81040]
	39484.95	(0.05)	9(8, 2) - 8(8, 1)	[81040]
	31170.88	(0.05)	14(1,14) - 14(1,13)	[81040]
	27049.03	(0.05)	6(2, 4) - 5(2, 3)	[81040]
	31505.40	(0.05)	7(1, 6) - 6(1, 5)	[81040]
	31730.15	(0.05)	7(2, 5) - 6(2, 4)	[81040]
	30990.28	(0.05)	7(3, 4) - 6(3, 3)	[81040]
	30789.37	(0.05)	7(4, 3) - 6(4, 2)	[81040]
	30739.40	(0.05)	7(5, 2) - 6(5, 1)	[81040]
	30715.26	(0.05)	7(6, 1) - 6(6, 0)	[81040]
	33208.63	(0.05)	8(0, 8) - 7(0, 7)	[81040]
	32940.61	(0.05)	8(1, 8) - 7(1, 7)	[81040]
	34620.71	(0.05)	8(2, 7) - 7(2, 6)	[81040]
	35211.17	(0.05)	8(3, 6) - 7(3, 5)	[81040]
	35216.21	(0.05)	8(4, 5) - 7(4, 4)	[81040]
	35157.05	(0.05)	8(5, 4) - 7(5, 3)	[81040]
	35121.36	(0.05)	8(6, 3) - 7(6, 2)	[81040]
	35100.06	(0.05)	8(7, 2) - 7(7, 1)	[81040]
	39930.28	(0.05)	9(1, 8) - 8(1, 7)	[81040]
	38823.52	(0.05)	9(2, 8) - 8(2, 7)	[81040]
	39711.28	(0.05)	9(4, 5) - 8(4, 4)	[81040]
	39586.95	(0.05)	9(5, 4) - 8(5, 3)	[81040]
	39534.75	(0.05)	9(6, 3) - 8(6, 2)	[81040]
	39504.46	(0.05)	9(7, 2) - 8(7, 1)	[81040]
	39484.95	(0.05)	9(8, 1) - 8(8, 0)	[81040]
	28419.25	(0.05)	13(1,13) - 13(1,12)	[81040]
	33855.08	(0.05)	15(1,15) - 15(1,14)	[81040]
	36488.56	(0.05)	16(1,16) - 16(1,15)	[81040]
	29237.94	(0.05)	16(2,15) - 16(2,14)	[81040]
	35430.35	(0.05)	18(2,17) - 18(2,16)	[81040]
	35519.32	(0.05)	21(3,19) - 21(3,18)	[81040]
	29579.64	(0.05)	23(4,20) - 23(4,19)	[81040]
	39085.92	(0.05)	17(1,17) - 17(1,16)	[81040]
	32401.74	(0.05)	17(2,16) - 17(2,15)	[81040]
	31945.10	(0.05)	20(3,18) - 20(3,17)	[81040]
	38918.56	(0.05)	22(3,20) - 22(3,19)	[81040]
	33737.67	(0.05)	24(4,21) - 24(4,20)	[81040]
	22121.64	(0.05)	5(2, 4) - 4(2, 3)	[81040]
	22351.20	(0.05)	5(3, 3) - 4(3, 2)	[81040]
	27615.99	(0.05)	6(1, 5) - 5(1, 4)	[81040]
	26845.79	(0.05)	6(3, 4) - 5(3, 3)	[81040]
	26819.44	(0.05)	6(4, 3) - 5(4, 2)	[81040]
	29349.57	(0.05)	7(0, 7) - 6(0, 6)	[81040]
	31968.30	(0.05)	7(1, 6) - 6(1, 5)	[81040]
	32509.20	(0.05)	7(2, 5) - 6(2, 4)	[81040]
	31657.94	(0.05)	7(3, 4) - 6(3, 3)	[81040]
	31347.34	(0.05)	7(4, 3) - 6(4, 2)	[81040]
	31238.42	(0.05)	7(6, 1) - 6(6, 0)	[81040]
	33080.24	(0.05)	8(1, 8) - 7(1, 7)	[81040]
	35017.86	(0.05)	8(2, 7) - 7(2, 6)	[81040]
	35811.53	(0.05)	8(3, 6) - 7(3, 5)	[81040]
	35856.23	(0.05)	8(4, 5) - 7(4, 4)	[81040]



TABLE 74.3. Microwave spectrum of spiro[2.4]hepta-4,6-diene — Continued

C₇H₈


Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$ - $J''(K_{-1}, K_{+1})$	Ref.
	35727.11	(0.05)	8(6, 3) - 7(6, 2)	[81040]
	35696.75	(0.05)	8(7, 2) - 7(7, 1)	[81040]
	37224.77	(0.05)	9(0, 9) - 8(0, 8)	[81040]
	39223.87	(0.05)	9(2, 8) - 8(2, 7)	[81040]
	30171.70	(0.05)	18(3,16) - 18(3,15)	[81040]
	22920.91	(0.05)	5(2, 3) - 4(2, 2)	[81040]
	22408.54	(0.05)	5(3, 2) - 4(3, 1)	[81040]
	27718.42	(0.05)	6(2, 4) - 5(2, 3)	[81040]
	26995.19	(0.05)	6(3, 3) - 5(3, 2)	[81040]
	26824.40	(0.05)	6(4, 2) - 5(4, 1)	[81040]
	29043.83	(0.05)	7(1, 7) - 6(1, 6)	[81040]
	30764.07	(0.05)	7(2, 6) - 6(2, 5)	[81040]
	31336.10	(0.05)	7(3, 5) - 6(3, 4)	[81040]
	31330.72	(0.05)	7(4, 4) - 6(4, 3)	[81040]
	31238.42	(0.05)	7(6, 2) - 6(6, 1)	[81040]
	33283.26	(0.05)	8(0, 8) - 7(0, 7)	[81040]
	36188.75	(0.05)	8(1, 7) - 7(1, 6)	[81040]
	37245.39	(0.05)	8(2, 6) - 7(2, 5)	[81040]
	36412.11	(0.05)	8(3, 5) - 7(3, 4)	[81040]
	35901.18	(0.05)	8(4, 4) - 7(4, 3)	[81040]
	35727.14	(0.05)	8(6, 2) - 7(6, 1)	[81040]
	35696.75	(0.05)	8(7, 1) - 7(7, 0)	[81040]
	37097.54	(0.05)	9(1, 9) - 8(1, 8)	[81040]
	39031.78	(0.05)	16(1,16) - 16(1,15)	[81040]
	33482.75	(0.05)	22(4,19) - 22(4,18)	[81040]
CH ₂ CH ₂ CCHDCCHCH	22554.18	(0.05)	5(1, 4) - 4(1, 3)	[81040]
	22224.86	(0.05)	5(2, 3) - 4(2, 2)	[81040]
	21819.50	(0.05)	5(3, 2) - 4(3, 1)	[81040]
	21760.51	(0.05)	5(4, 1) - 4(4, 0)	[81040]
	26860.84	(0.05)	6(2, 4) - 5(2, 3)	[81040]
	28565.10	(0.05)	7(1, 7) - 6(1, 6)	[81040]
	30100.51	(0.05)	7(2, 6) - 6(2, 5)	[81040]
	30542.47	(0.05)	7(3, 5) - 6(3, 4)	[81040]
	30523.47	(0.05)	7(4, 4) - 6(4, 3)	[81040]
	30453.42	(0.05)	7(6, 2) - 6(6, 1)	[81040]
	32819.45	(0.05)	8(0, 8) - 7(0, 7)	[81040]
	35473.30	(0.05)	8(1, 7) - 7(1, 6)	[81040]
	36147.38	(0.05)	8(2, 6) - 7(2, 5)	[81040]
	35304.26	(0.05)	8(3, 5) - 7(3, 4)	[81040]
	34946.40	(0.05)	8(4, 4) - 7(4, 3)	[81040]
	34823.15	(0.05)	8(6, 2) - 7(6, 1)	[81040]
	36519.90	(0.05)	9(1, 9) - 8(1, 8)	[81040]
	39168.59	(0.05)	9(7, 3) - 8(7, 2)	[81040]
	39147.98	(0.05)	9(8, 2) - 8(8, 1)	[81040]
	32101.14	(0.05)	14(1,14) - 14(1,13)	[81040]
	36869.88	(0.05)	21(3,19) - 21(3,18)	[81040]
	21610.55	(0.05)	5(2, 4) - 4(2, 3)	[81040]
	21783.96	(0.05)	5(3, 3) - 4(3, 2)	[81040]
	21759.91	(0.05)	5(4, 2) - 4(4, 1)	[81040]
	26945.59	(0.05)	6(1, 5) - 5(1, 4)	[81040]
	28936.14	(0.05)	7(0, 7) - 6(0, 6)	[81040]
	30532.06	(0.05)	7(4, 3) - 6(4, 2)	[81040]
	30453.42	(0.05)	7(6, 1) - 6(6, 0)	[81040]
	30746.27	(0.05)	7(3, 4) - 6(3, 3)	[81040]
	31258.28	(0.05)	7(1, 6) - 6(1, 5)	[81040]
	31515.20	(0.05)	7(2, 5) - 6(2, 4)	[81040]
	32551.90	(0.05)	8(1, 8) - 7(1, 7)	[81040]
	34293.70	(0.05)	8(2, 7) - 7(2, 6)	[81040]
	34915.19	(0.05)	8(3, 6) - 7(3, 5)	[81040]
	34923.14	(0.05)	8(4, 5) - 7(4, 4)	[81040]
	34823.14	(0.05)	8(6, 3) - 7(6, 2)	[81040]
	36701.46	(0.05)	9(0, 9) - 8(0, 8)	[81040]
	39577.90	(0.05)	9(1, 8) - 8(1, 7)	[81040]
	39168.59	(0.05)	9(7, 2) - 8(7, 1)	[81040]
	39147.98	(0.05)	9(8, 1) - 8(8, 0)	[81040]
	33495.16	(0.05)	17(2,16) - 17(2,15)	[81040]
	35312.83	(0.05)	24(4,21) - 24(4,20)	[81040]

Table 75.1. Molecular constants of bicyclo[2.2.1]hept-2-ene (norbornene).

Parameter	Value
<u>Rotational Constants</u> [present]	
A (MHz)	3923.773(21)
B (MHz)	3432.3668(30)
C (MHz)	3014.9251(28)
<u>Electric Dipole Moment</u> [77037]	
μ_a (D)	0.327(5)
μ_c (D)	0.00(1)

TABLE 75.2. Microwave spectrum of bicyclo[2.2.1]hept-2-ene

C₇H₁₀


Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
$\text{CH}(\text{CH}_2)\text{CHCHCH}_2\text{CH}_2$ 	26652.52	(0.10)	4(2, 2) - 3(2, 1)	[77037]
	30757.28	(0.10)	5(1, 5) - 4(1, 4)	[77037]
	30777.69	(0.10)	5(0, 5) - 4(0, 4)	[77037]
	31852.30	(0.10)	5(2, 4) - 4(2, 3)	[77037]
	32161.51	(0.10)	5(1, 4) - 4(1, 3)	[77037]
	32494.14	(0.10)	5(3, 3) - 4(3, 2)	[77037]
	32620.70	(0.10)	5(4, 2) - 4(4, 1)	[77037]
	32710.10	(0.10)	5(4, 1) - 4(4, 0)	[77037]
	33174.48	(0.10)	5(3, 2) - 4(3, 1)	[77037]
	33221.66	(0.10)	5(2, 3) - 4(2, 2)	[77037]
	36793.50	(0.10)	6(1, 6) - 5(1, 5)	[77037]
	36799.26	(0.10)	6(0, 6) - 5(0, 5)	[77037]
	37974.58	(0.10)	6(2, 5) - 5(2, 4)	[77037]
	39151.62	(0.10)	6(5, 2) - 5(5, 1)	[77037]
	39176.28	(0.10)	6(5, 1) - 5(5, 0)	[77037]
	39182.84	(0.10)	6(4, 3) - 5(4, 2)	[77037]
	39513.50	(0.10)	6(4, 2) - 5(4, 1)	[77037]
	39527.91	(0.10)	6(2, 4) - 5(2, 3)	[77037]

Table 76.1. Molecular constants of the ground state of 1,3-cycloheptadiene.

Parameter	Value [present work]
A'' (MHz)	3419.3116(25)
B'' (MHz)	3297.4144(24)
C'' (MHz)	1799.9643(25)
τ_1 (kHz)	-26.2544(3447)
τ_2 (kHz)	-6.38596(9408)
τ_3^a (kHz)	1503.(18)
τ_{aaaa} (kHz)	-3.039(155)
τ_{bbbb} (kHz)	-2.4872(826)
τ_{cccc} (kHz)	-0.602(81)
H _J (Hz)	0 ^b
H _{JK} (Hz)	0.48689(8713)
H _{KJ} (Hz)	-0.99682(21785)
H _K (Hz)	0.6188(1481)
h _J (Hz)	0.03532(479)
h _{JK} (Hz)	0 ^b
h _K (Hz)	0 ^b
<u>Electric Dipole Moments</u> [79034]	
μ_b (D)	0.734(3)
μ_c (D)	0.0975(5)

^aValue fixed by setting R_g = 0.^bFixed at zero.

Table 76.2. Molecular constants of the vibrational states of 1,3-cycloheptadiene. [79034]

Parameter	A	B	C
A (MHz)	3417.646(3)	3416.607(4)	3415.379(5)
B (MHz)	3309.165(3)	3314.519(4)	3319.787(5)
C (MHz)	1809.368(3)	1813.785(4)	1818.154(3)
Δ_J (kHz)	0.70554(2200)	0.8277(3200)	0.68068(3400)
Δ_{JK} (kHz)	-1.6432(99)	-1.5257(920)	-1.0558(1600)
Δ_K (kHz)	1.0895(110)	0.8247(770)	0.4765(1400)
δ_J (kHz)	-0.01476(840)	-0.052891(4900)	-0.027142(4500)
δ_K (kHz)	7.5148(840)	4.0077(9200)	-0.43(170)
	D	E	
A (MHz)	3413.71(10)	3412.77(8)	
B (MHz)	3324.53(10)	3328.31(8)	
C (MHz)	1821.94(3)	1825.36(3)	

TABLE 76.3. Microwave spectrum of 1,3-cycloheptadiene

C₇H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_-,K_+)$ - $J''(K_-,K_+)$	Vib. state	Ref.
CHCHCHCHCH ₂ CH ₂ CH ₂	7711.75	(0.10)	4(2,2) - 4(1,3)		[79034]
	7760.95	(0.10)	3(1,2) - 3(0,3)		[79034]
	7796.20	(0.10)	3(2,2) - 3(1,3)		[79034]
	7815.10	(0.10)	4(3,2) - 4(2,3)		[79034]
	7852.48	(0.10)	5(4,2) - 5(3,3)		[79034]
	8690.06	(0.10)	2(0,2) - 1(1,1)		[79034]
	8819.15	(0.10)	2(1,2) - 1(0,1)		[79034]
	10820.50	(0.10)	7(4,3) - 7(3,4)		[79034]
	10882.70	(0.10)	5(2,3) - 5(1,4)		[79034]
	10894.40	(0.10)	4(1,3) - 4(0,4)		[79034]
	10896.30	(0.10)	4(2,3) - 4(1,4)		[79034]
	12057.82	(0.10)	2(2,1) - 1(1,0)		[79034]
	12353.47	(0.10)	3(0,3) - 2(1,2)		[79034]
	12361.02	(0.10)	3(1,3) - 2(0,2)		[79034]
	27223.77	(0.10)	40(31,9) - 40(30,10)		[79034]
	27507.17	(0.10)	39(30,9) - 39(29,10)		[79034]
	27534.32	(0.10)	40(32,9) - 40(31,10)		[79034]
	27715.34	(0.10)	39(31,9) - 39(30,10)		[79034]
	27752.35	(0.10)	38(29,9) - 38(28,10)		[79034]
	27965.97	(0.10)	37(28,9) - 37(27,10)		[79034]
	28054.69	(0.10)	37(29,9) - 37(28,10)		[79034]
	28060.68	(0.10)	5(3,2) - 4(4,1)		[79034]
	28153.58	(0.10)	36(27,9) - 36(26,10)		[79034]
	28160.30	(0.10)	4(4,0) - 3(3,1)		[79034]
	28209.85	(0.10)	36(28,9) - 36(27,10)		[79034]
	28319.32	(0.10)	35(26,9) - 35(25,10)		[79034]
	28354.44	(0.10)	35(27,9) - 35(26,10)		[79034]
	28466.39	(0.10)	34(25,9) - 34(24,10)		[79034]
	28487.88	(0.10)	34(26,9) - 34(25,10)		[79034]
	28597.74	(0.10)	33(24,9) - 33(23,10)		[79034]
	28610.62	(0.10)	33(25,9) - 33(24,10)		[79034]
	28715.11	(0.10)	32(23,9) - 32(22,10)		[79034]
	28722.69	(0.10)	32(24,9) - 32(23,10)		[79034]
	28820.47	(0.10)	31(22,9) - 31(21,10)		[79034]
	28824.82	(0.10)	31(23,9) - 31(22,10)		[79034]
	28914.96	(0.10)	30(21,9) - 30(20,10)		[79034]
	28917.43	(0.10)	30(22,9) - 30(21,10)		[79034]
	28999.77	(0.10)	29(20,9) - 29(19,10)		[79034]
	29001.06	(0.10)	29(21,9) - 29(20,10)		[79034]
	29075.90	(0.10)	28(19,9) - 28(18,10)		[79034]
	29076.56	(0.10)	28(20,9) - 28(19,10)		[79034]
	29143.86	(0.10)	27(18,9) - 27(17,10)		[79034]
	29144.15	(0.10)	27(19,9) - 27(18,10)		[79034]
	29204.67	(0.10)	26(18,9) - 26(17,10)		[79034]
	29258.75	(0.10)	25(16,9) - 25(15,10)		[79034]
	29306.87	(0.10)	24(15,9) - 24(14,10)		[79034]
	29349.38	(0.10)	23(14,9) - 23(13,10)		[79034]
	29384.66	(0.10)	6(2,4) - 5(3,3)		[79034]
	29386.88	(0.10)	22(13,9) - 22(12,10)		[79034]
	29392.25	(0.10)	6(3,4) - 5(2,3)		[79034]
29419.82	(0.10)	21(12,9) - 21(11,10)		[79034]	
29448.60	(0.10)	20(11,9) - 20(10,10)		[79034]	
29473.57	(0.10)	19(11,9) - 19(10,10)		[79034]	
29495.20	(0.10)	18(10,9) - 18(9,10)		[79034]	
29513.63	(0.10)	17(9,9) - 17(8,10)		[79034]	
29518.40	(0.10)	5(4,2) - 4(3,1)		[79034]	
29529.37	(0.10)	16(8,9) - 16(7,10)		[79034]	
29542.62	(0.10)	15(6,9) - 15(5,10)		[79034]	
29553.79	(0.10)	14(6,9) - 14(5,10)		[79034]	
29563.08	(0.10)	13(5,9) - 13(4,10)		[79034]	
29570.68	(0.10)	12(3,9) - 12(2,10)		[79034]	
29576.70	(0.10)	11(2,9) - 11(1,10)		[79034]	
29581.56	(0.10)	10(1,9) - 10(0,10)		[79034]	
29870.60	(0.10)	7(2,6) - 6(1,5)		[79034]	
29870.60	(0.10)	7(1,6) - 6(2,5)		[79034]	
30355.98	(0.10)	8(1,8) - 7(0,7)		[79034]	
32200.40	(0.10)	30(21,10) - 30(20,11)		[79034]	
32317.67	(0.10)	28(19,10) - 28(18,11)		[79034]	

TABLE 76.3. Microwave spectrum of 1,3-cycloheptadiene — Continued

C₇H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$	$- J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	32412.78	(0.10)	26(17,10)	- 26(16,11)		[79034]
	32489.02	(0.10)	24(15,10)	- 24(14,11)		[79034]
	32549.22	(0.10)	22(13,10)	- 22(12,11)		[79034]
	32595.97	(0.10)	20(11,10)	- 20(10,11)		[79034]
	32631.62	(0.10)	18(9,10)	- 18(8,11)		[79034]
	32654.58	(0.10)	6(4,3)	- 5(3,2)		[79034]
	32658.05	(0.10)	16(7,10)	- 16(6,11)		[79034]
	32677.12	(0.10)	14(5,10)	- 14(4,11)		[79034]
	32690.44	(0.10)	12(3,10)	- 12(2,11)		[79034]
	32695.43	(0.10)	11(2,10)	- 11(1,11)		[79034]
	32879.59	(0.10)	5(5,1)	- 4(4,0)		[79034]
	32986.07	(0.10)	7(2,5)	- 6(3,4)		[79034]
	32986.37	(0.10)	7(3,5)	- 6(2,4)		[79034]
	33470.25	(0.10)	8(1,7)	- 7(2,6)		[79034]
	33955.80	(0.10)	9(1,9)	- 8(0,8)		[79034]
	34249.51	(0.10)	6(4,2)	- 5(5,1)		[79034]
	34668.47	(0.10)	4(3,2)	- 3(0,3)		[79034]
	34755.19	(0.10)	5(5,0)	- 4(4,1)		[79034]
	35425.94	(0.10)	30(20,11)	- 30(19,12)		[79034]
	35515.87	(0.10)	28(18,11)	- 28(17,12)		[79034]
	35589.38	(0.10)	26(16,11)	- 26(15,12)		[79034]
	35648.63	(0.10)	24(14,11)	- 24(13,12)		[79034]
	35695.75	(0.10)	22(12,11)	- 22(11,12)		[79034]
	35732.74	(0.10)	20(10,11)	- 20(9,12)		[79034]
	35761.09	(0.10)	18(8,11)	- 18(7,12)		[79034]
	35782.40	(0.10)	16(6,11)	- 16(5,12)		[79034]
	35797.97	(0.10)	14(4,11)	- 14(3,12)		[79034]
	35809.10	(0.10)	12(2,11)	- 12(1,12)		[79034]
	36096.96	(0.10)	7(3,4)	- 6(4,3)		[79034]
	36119.72	(0.10)	7(4,4)	- 6(3,3)		[79034]
	36536.77	(0.10)	6(5,2)	- 5(4,1)		[79034]
	36585.11	(0.10)	8(2,6)	- 7(3,5)		[79034]
	37069.86	(0.10)	9(1,8)	- 8(2,7)		[79034]
	37392.06	(0.10)	5(4,1)	- 4(3,2)		[79034]
	37555.55	(0.10)	10(1,10)	- 9(0,9)		[79034]
	38616.64	(0.10)	30(18,12)	- 30(17,13)		[79034]
	38688.02	(0.10)	28(16,12)	- 28(15,13)		[79034]
	38746.71	(0.10)	26(14,12)	- 26(13,13)		[79034]
	38794.39	(0.10)	24(12,12)	- 24(11,13)		[79034]
	38832.63	(0.10)	22(10,12)	- 22(9,13)		[79034]
	38862.83	(0.10)	20(8,12)	- 20(7,13)		[79034]
	38886.32	(0.10)	18(6,12)	- 18(5,13)		[79034]
	38904.11	(0.10)	16(4,12)	- 16(3,13)		[79034]
	38917.41	(0.10)	14(2,12)	- 14(1,13)		[79034]
	38922.75	(0.10)	13(1,12)	- 13(0,13)		[79034]
	39001.22	(0.10)	7(4,3)	- 6(5,2)		[79034]
	39520.37	(0.10)	7(5,3)	- 6(4,2)		[79034]
	39702.15	(0.10)	8(3,5)	- 7(4,4)		[79034]
	39875.52	(0.10)	6(6,1)	- 5(5,0)		[79034]
	7630.95	(0.10)	5(3,2)	- 5(2,3)	1v a	[79034]
	7705.91	(0.10)	4(2,2)	- 4(1,3)	1v a	[79034]
	7773.68	(0.10)	3(2,2)	- 3(1,3)	1v a	[79034]
	7788.92	(0.10)	4(3,2)	- 4(2,3)	1v a	[79034]
	7819.06	(0.10)	5(4,2)	- 5(3,3)	1v a	[79034]
	7870.95	(0.10)	6(5,2)	- 6(4,3)	1v a	[79034]
	8731.65	(0.10)	2(0,2)	- 1(1,1)	1v a	[79034]
	8845.75	(0.10)	2(1,2)	- 1(0,1)	1v a	[79034]
	8999.85	(0.10)	12(11,2)	- 12(10,3)	1v a	[79034]
	10810.25	(0.10)	7(4,3)	- 7(3,4)	1v a	[79034]
	10836.50	(0.10)	9(7,3)	- 9(6,4)	1v a	[79034]
	10863.22	(0.10)	5(3,3)	- 5(2,4)	1v a	[79034]
	10867.05	(0.10)	4(1,3)	- 4(0,4)	1v a	[79034]
	10868.40	(0.10)	4(2,3)	- 4(1,4)	1v a	[79034]
	12062.30	(0.10)	2(2,1)	- 1(1,0)	1v a	[79034]
	12406.58	(0.10)	3(0,3)	- 2(1,2)	1v a	[79034]
	12412.50	(0.10)	3(1,3)	- 2(0,2)	1v a	[79034]
	26884.03	(0.10)	7(1,7)	- 6(0,6)	1v a	[79034]

TABLE 76.3. Microwave spectrum of 1,3-cycloheptadiene — Continued

C₇H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_-,K_+) - J''(K_-,K_+)$	Vib. state	Ref.
	27654.59	(0.10)	40(31, 9) - 40(30,10)	1v a	[79034]
	27868.24	(0.10)	40(32, 9) - 40(31,10)	1v a	[79034]
	28071.43	(0.10)	38(29, 9) - 38(28,10)	1v a	[79034]
	28164.04	(0.10)	38(30, 9) - 38(29,10)	1v a	[79034]
	28216.14	(0.10)	4(4, 0) - 3(3, 1)	1v a	[79034]
	28240.20	(0.10)	37(28, 9) - 37(27,10)	1v a	[79034]
	28299.65	(0.10)	37(29, 9) - 37(28,10)	1v a	[79034]
	28388.58	(0.10)	36(27, 9) - 36(26,10)	1v a	[79034]
	28426.05	(0.10)	36(28, 9) - 36(27,10)	1v a	[79034]
	28519.71	(0.10)	35(26, 9) - 35(25,10)	1v a	[79034]
	28543.03	(0.10)	35(27, 9) - 35(26,10)	1v a	[79034]
	28636.15	(0.10)	34(25, 9) - 34(24,10)	1v a	[79034]
	28650.42	(0.10)	34(26, 9) - 34(25,10)	1v a	[79034]
	28740.23	(0.10)	33(24, 9) - 33(23,10)	1v a	[79034]
	28748.65	(0.10)	33(25, 9) - 33(24,10)	1v a	[79034]
	28833.20	(0.10)	32(23, 9) - 32(22,10)	1v a	[79034]
	28838.16	(0.10)	32(24, 9) - 32(23,10)	1v a	[79034]
	28916.41	(0.10)	31(22, 9) - 31(21,10)	1v a	[79034]
	28919.26	(0.10)	31(23, 9) - 31(22,10)	1v a	[79034]
	28990.91	(0.10)	30(21, 9) - 30(20,10)	1v a	[79034]
	28992.52	(0.10)	30(22, 9) - 30(21,10)	1v a	[79034]
	29057.77	(0.10)	29(20, 9) - 29(19,10)	1v a	[79034]
	29058.59	(0.10)	29(21, 9) - 29(20,10)	1v a	[79034]
	29170.90	(0.10)	27(18, 9) - 27(17,10)	1v a	[79034]
	29218.32	(0.10)	26(18, 9) - 26(17,10)	1v a	[79034]
	29260.48	(0.10)	25(16, 9) - 25(15,10)	1v a	[79034]
	29297.82	(0.10)	24(15, 9) - 24(14,10)	1v a	[79034]
	29330.82	(0.10)	23(14, 9) - 23(13,10)	1v a	[79034]
	29359.78	(0.10)	22(13, 9) - 22(12,10)	1v a	[79034]
	29385.08	(0.10)	21(12, 9) - 21(11,10)	1v a	[79034]
	29407.05	(0.10)	20(11, 9) - 20(10,10)	1v a	[79034]
	29426.16	(0.10)	19(11, 9) - 19(10,10)	1v a	[79034]
	29442.52	(0.10)	18(10, 9) - 18(9,10)	1v a	[79034]
	29456.38	(0.10)	17(9, 9) - 17(8,10)	1v a	[79034]
	29468.20	(0.10)	16(8, 9) - 16(7,10)	1v a	[79034]
	29477.95	(0.10)	6(2, 4) - 5(3, 3)	1v a	[79034]
	29478.00	(0.10)	15(6, 9) - 15(5,10)	1v a	[79034]
	29483.42	(0.10)	6(3, 4) - 5(2, 3)	1v a	[79034]
	29486.21	(0.10)	14(6, 9) - 14(5,10)	1v a	[79034]
	29492.93	(0.10)	13(5, 9) - 13(4,10)	1v a	[79034]
	29498.37	(0.10)	12(3, 9) - 12(2,10)	1v a	[79034]
	29515.78	(0.10)	5(4, 2) - 4(3, 1)	1v a	[79034]
	29990.37	(0.10)	7(2, 6) - 6(1, 5)	1v a	[79034]
	30502.68	(0.10)	8(1, 8) - 7(0, 7)	1v a	[79034]
	32235.34	(0.10)	30(20,10) - 30(19,11)	1v a	[79034]
	32326.85	(0.10)	28(18,10) - 28(17,11)	1v a	[79034]
	32400.62	(0.10)	26(16,10) - 26(15,11)	1v a	[79034]
	32459.23	(0.10)	24(15,10) - 24(14,11)	1v a	[79034]
	32499.87	(0.10)	6(3, 3) - 5(4, 2)	1v a	[79034]
	32505.04	(0.10)	22(12,10) - 22(11,11)	1v a	[79034]
	32540.24	(0.10)	20(10,10) - 20(9,11)	1v a	[79034]
	32566.71	(0.10)	18(8,10) - 18(7,11)	1v a	[79034]
	32585.96	(0.10)	16(6,10) - 16(5,11)	1v a	[79034]
	32599.64	(0.10)	14(4,10) - 14(3,11)	1v a	[79034]
	32608.81	(0.10)	12(2,10) - 12(1,11)	1v a	[79034]
	32708.34	(0.10)	6(4, 3) - 5(3, 2)	1v a	[79034]
	32846.70	(0.10)	5(5, 1) - 4(4, 0)	1v a	[79034]
	33097.70	(0.10)	7(3, 5) - 6(2, 4)	1v a	[79034]
	33608.91	(0.10)	8(2, 7) - 7(1, 6)	1v a	[79034]
	34121.29	(0.10)	9(1, 9) - 8(0, 8)	1v a	[79034]
	34513.14	(0.10)	6(4, 2) - 5(5, 1)	1v a	[79034]
	34824.10	(0.10)	5(5, 0) - 4(4, 1)	1v a	[79034]
	35432.40	(0.10)	30(20,11) - 30(19,12)	1v a	[79034]
	35501.69	(0.10)	28(18,11) - 28(17,12)	1v a	[79034]
	35557.74	(0.10)	26(16,11) - 26(15,12)	1v a	[79034]
	35602.50	(0.10)	24(14,11) - 24(13,12)	1v a	[79034]
	35637.67	(0.10)	22(12,11) - 22(11,12)	1v a	[79034]

TABLE 76.3. Microwave spectrum of 1,3-cycloheptadiene — Continued

C₇H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$ - $J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	35664.85	(0.10)	20(10,11) - 20(9,12)	1v a	[79034]
	35685.33	(0.10)	18(8,11) - 18(7,12)	1v a	[79034]
	35700.37	(0.10)	16(6,11) - 16(5,12)	1v a	[79034]
	35711.02	(0.10)	14(4,11) - 14(3,12)	1v a	[79034]
	35718.39	(0.10)	12(2,11) - 12(1,12)	1v a	[79034]
	36202.03	(0.10)	7(3, 4) - 6(4, 3)	1v a	[79034]
	36218.33	(0.10)	7(4, 4) - 6(3, 3)	1v a	[79034]
	36512.35	(0.10)	6(5, 2) - 5(4, 1)	1v a	[79034]
	36715.77	(0.10)	8(3, 6) - 7(2, 5)	1v a	[79034]
	37227.52	(0.10)	9(2, 8) - 8(1, 7)	1v a	[79034]
	37520.08	(0.10)	5(4, 1) - 4(3, 2)	1v a	[79034]
	37739.89	(0.10)	10(1,10) - 9(0, 9)	1v a	[79034]
	38601.35	(0.10)	30(18,12) - 30(17,13)	1v a	[79034]
	38699.61	(0.10)	26(15,12) - 26(14,13)	1v a	[79034]
	38734.80	(0.10)	24(12,12) - 24(11,13)	1v a	[79034]
	38762.63	(0.10)	22(10,12) - 22(9,13)	1v a	[79034]
	38784.19	(0.10)	20(8,12) - 20(7,13)	1v a	[79034]
	38800.51	(0.10)	18(6,12) - 18(5,13)	1v a	[79034]
	38812.55	(0.10)	16(4,12) - 16(3,13)	1v a	[79034]
	38821.28	(0.10)	14(2,12) - 14(1,13)	1v a	[79034]
	38824.45	(0.10)	13(1,12) - 13(0,13)	1v a	[79034]
	39141.45	(0.10)	7(4, 3) - 6(5, 2)	1v a	[79034]
	39226.65	(0.10)	5(5, 1) - 4(2, 2)	1v a	[79034]
	39830.05	(0.10)	6(6, 1) - 5(5, 0)	1v a	[79034]
	7701.90	(0.10)	4(2, 2) - 4(1, 3)	1v b	[79034]
	7761.96	(0.10)	3(2, 2) - 3(1, 3)	1v b	[79034]
	7775.46	(0.10)	4(3, 2) - 4(2, 3)	1v b	[79034]
	7802.20	(0.10)	5(4, 2) - 5(3, 3)	1v b	[79034]
	8750.88	(0.10)	2(0, 2) - 1(1, 1)	1v b	[79034]
	8857.92	(0.10)	2(1, 2) - 1(0, 1)	1v b	[79034]
	10842.35	(0.10)	6(4, 3) - 6(3, 4)	1v b	[79034]
	10844.70	(0.10)	5(2, 3) - 5(1, 4)	1v b	[79034]
	10852.50	(0.10)	4(1, 3) - 4(0, 4)	1v b	[79034]
	12063.66	(0.10)	2(2, 1) - 1(1, 0)	1v b	[79034]
	26943.59	(0.10)	7(1, 7) - 6(0, 6)	1v b	[79034]
	28241.40	(0.10)	4(4, 0) - 3(3, 1)	1v b	[79034]
	28597.62	(0.10)	35(26, 9) - 35(25,10)	1v b	[79034]
	28611.21	(0.10)	35(27, 9) - 35(26,10)	1v b	[79034]
	28705.93	(0.10)	34(26, 9) - 34(25,10)	1v b	[79034]
	28868.49	(0.10)	32(23, 9) - 32(22,10)	1v b	[79034]
	28941.15	(0.10)	31(22, 9) - 31(21,10)	1v b	[79034]
	28942.65	(0.10)	31(23, 9) - 31(22,10)	1v b	[79034]
	29006.40	(0.10)	30(21, 9) - 30(20,10)	1v b	[79034]
	29007.25	(0.10)	30(22, 9) - 30(21,10)	1v b	[79034]
	29164.90	(0.10)	27(18, 9) - 27(17,10)	1v b	[79034]
	29207.00	(0.10)	26(17, 9) - 26(16,10)	1v b	[79034]
	29244.31	(0.10)	25(16, 9) - 25(15,10)	1v b	[79034]
	29277.74	(0.10)	24(15, 9) - 24(14,10)	1v b	[79034]
	29332.94	(0.10)	22(13, 9) - 22(12,10)	1v b	[79034]
	29355.56	(0.10)	21(12, 9) - 21(11,10)	1v b	[79034]
	29375.50	(0.10)	20(11, 9) - 20(10,10)	1v b	[79034]
	29392.35	(0.10)	19(10, 9) - 19(9,10)	1v b	[79034]
	29407.15	(0.10)	18(9, 9) - 18(8,10)	1v b	[79034]
	29419.70	(0.10)	17(8, 9) - 17(7,10)	1v b	[79034]
	29430.41	(0.10)	16(7, 9) - 16(6,10)	1v b	[79034]
	29439.34	(0.10)	15(6, 9) - 15(5,10)	1v b	[79034]
	29446.79	(0.10)	14(5, 9) - 14(4,10)	1v b	[79034]
	29453.00	(0.10)	13(4, 9) - 13(3,10)	1v b	[79034]
	29457.89	(0.10)	12(3, 9) - 12(2,10)	1v b	[79034]
	29462.00	(0.10)	11(2, 9) - 11(1,10)	1v b	[79034]
	29465.10	(0.10)	10(1, 9) - 10(0,10)	1v b	[79034]
	29511.70	(0.10)	5(4, 2) - 4(3, 1)	1v b	[79034]
	29520.08	(0.10)	6(2, 4) - 5(3, 3)	1v b	[79034]
	29524.58	(0.10)	6(3, 4) - 5(2, 3)	1v b	[79034]
	30045.57	(0.10)	7(2, 6) - 6(1, 5)	1v b	[79034]
	30571.12	(0.10)	8(1, 8) - 7(0, 7)	1v b	[79034]
	32309.89	(0.10)	28(18,10) - 28(17,11)	1v b	[79034]

TABLE 76.3. Microwave spectrum of 1,3-cycloheptadiene — Continued

C₇H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	32375.36	(0.10)	26(16,10) - 26(15,11)	1v b	[79034]
	32427.93	(0.10)	24(14,10) - 24(13,11)	1v b	[79034]
	32469.13	(0.10)	22(12,10) - 22(11,11)	1v b	[79034]
	32500.70	(0.10)	20(11,10) - 20(10,11)	1v b	[79034]
	32524.85	(0.10)	18(9,10) - 18(8,11)	1v b	[79034]
	32542.42	(0.10)	16(7,10) - 16(6,11)	1v b	[79034]
	32547.52	(0.10)	6(3, 3) - 5(4, 2)	1v b	[79034]
	32555.04	(0.10)	14(5,10) - 14(4,11)	1v b	[79034]
	32563.64	(0.10)	12(3,10) - 12(2,11)	1v b	[79034]
	32732.16	(0.10)	6(4, 3) - 5(3, 2)	1v b	[79034]
	32827.70	(0.10)	5(5, 1) - 4(4, 0)	1v b	[79034]
	33148.39	(0.10)	7(2, 5) - 6(3, 4)	1v b	[79034]
	34198.53	(0.10)	9(1, 9) - 8(0, 8)	1v b	[79034]
	34633.90	(0.10)	6(4, 2) - 5(5, 1)	1v b	[79034]
	35243.50	(0.10)	34(23,11) - 34(22,12)	1v b	[79034]
	35290.93	(0.10)	33(22,11) - 33(21,12)	1v b	[79034]
	35334.35	(0.10)	32(21,11) - 32(20,12)	1v b	[79034]
	35409.75	(0.10)	30(19,11) - 30(18,12)	1v b	[79034]
	35471.73	(0.10)	28(17,11) - 28(16,12)	1v b	[79034]
	35521.98	(0.10)	26(15,11) - 26(14,12)	1v b	[79034]
	35562.20	(0.10)	24(13,11) - 24(12,12)	1v b	[79034]
	35594.15	(0.10)	22(11,11) - 22(10,12)	1v b	[79034]
	35618.82	(0.10)	20(9,11) - 20(8,12)	1v b	[79034]
	35651.50	(0.10)	16(5,11) - 16(4,12)	1v b	[79034]
	35661.55	(0.10)	14(3,11) - 14(2,12)	1v b	[79034]
	35665.41	(0.10)	13(2,11) - 13(1,12)	1v b	[79034]
	36262.54	(0.10)	7(4, 4) - 6(3, 3)	1v b	[79034]
	36775.35	(0.10)	8(2, 6) - 7(3, 5)	1v b	[79034]
	37300.33	(0.10)	9(1, 8) - 8(2, 7)	1v b	[79034]
	37825.94	(0.10)	10(1,10) - 9(0, 9)	1v b	[79034]
	38712.40	(0.10)	22(10,12) - 22(9,13)	1v b	[79034]
	38732.22	(0.10)	20(8,12) - 20(7,13)	1v b	[79034]
	38758.79	(0.10)	16(5,12) - 16(4,13)	1v b	[79034]
	38767.04	(0.10)	14(2,12) - 14(1,13)	1v b	[79034]
	38770.23	(0.10)	13(1,12) - 13(0,13)	1v b	[79034]
	39180.18	(0.10)	5(5, 1) - 4(2, 2)	1v b	[79034]
	39203.80	(0.10)	7(4, 3) - 6(5, 2)	1v b	[79034]
	39803.85	(0.10)	6(6, 1) - 5(5, 0)	1v b	[79034]
	39879.30	(0.10)	8(3, 5) - 7(4, 4)	1v b	[79034]
	39880.00	(0.10)	8(4, 5) - 7(3, 4)	1v b	[79034]
	7727.95	(0.10)	3(1, 2) - 3(0, 3)	1v c	[79034]
	7749.85	(0.10)	3(2, 2) - 3(1, 3)	1v c	[79034]
	7785.38	(0.10)	5(4, 2) - 5(3, 3)	1v c	[79034]
	8769.83	(0.10)	2(0, 2) - 1(1, 1)	1v c	[79034]
	8869.83	(0.10)	2(1, 2) - 1(0, 1)	1v c	[79034]
	12064.40	(0.10)	2(2, 1) - 1(1, 0)	1v c	[79034]
	27002.62	(0.10)	7(1, 6) - 6(0, 6)	1v c	[79034]
	28400.04	(0.10)	5(3, 2) - 4(4, 1)	1v c	[79034]
	28673.59	(0.10)	35(27, 9) - 35(26,10)	1v c	[79034]
	28756.50	(0.10)	34(26, 9) - 34(25,10)	1v c	[79034]
	28829.60	(0.10)	33(24, 9) - 33(23,10)	1v c	[79034]
	28832.22	(0.10)	33(25, 9) - 33(24,10)	1v c	[79034]
	28899.55	(0.10)	32(23, 9) - 32(22,10)	1v c	[79034]
	28901.08	(0.10)	32(24, 9) - 32(23,10)	1v c	[79034]
	28962.71	(0.10)	31(22, 9) - 31(21,10)	1v c	[79034]
	28963.58	(0.10)	31(23, 9) - 31(22,10)	1v c	[79034]
	29019.80	(0.10)	30(21, 9) - 30(20,10)	1v c	[79034]
	29020.13	(0.10)	30(22, 9) - 30(21,10)	1v c	[79034]
	29117.12	(0.10)	28(19, 9) - 28(18,10)	1v c	[79034]
	29158.41	(0.10)	27(18, 9) - 27(17,10)	1v c	[79034]
	29195.36	(0.10)	26(17, 9) - 26(16,10)	1v c	[79034]
	29228.21	(0.10)	25(16, 9) - 25(15,10)	1v c	[79034]
	29257.48	(0.10)	24(15, 9) - 24(14,10)	1v c	[79034]
	29283.32	(0.10)	23(14, 9) - 23(13,10)	1v c	[79034]
	29306.00	(0.10)	22(13, 9) - 22(12,10)	1v c	[79034]
	29325.95	(0.10)	21(12, 9) - 21(11,10)	1v c	[79034]
	29399.86	(0.10)	15(6, 9) - 15(5,10)	1v c	[79034]

TABLE 76.3. Microwave spectrum of 1,3-cycloheptadiene — Continued

C₇H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	29406.50	(0.10)	14(5, 9) - 13(4, 10)	1v c	[79034]
	29411.91	(0.10)	13(5, 9) - 13(4, 10)	1v c	[79034]
	29416.48	(0.10)	12(3, 9) - 12(2, 10)	1v c	[79034]
	29422.84	(0.10)	10(2, 9) - 10(1, 10)	1v c	[79034]
	29506.50	(0.10)	5(4, 2) - 4(3, 1)	1v c	[79034]
	29561.40	(0.10)	6(2, 4) - 5(3, 3)	1v c	[79034]
	29565.12	(0.10)	6(3, 4) - 5(2, 3)	1v c	[79034]
	30100.11	(0.10)	7(1, 6) - 6(2, 5)	1v c	[79034]
	30638.91	(0.10)	8(1, 8) - 7(0, 7)	1v c	[79034]
	32397.15	(0.10)	24(14,10) - 24(13,11)	1v c	[79034]
	32433.48	(0.10)	22(12,10) - 22(11,11)	1v c	[79034]
	32461.55	(0.10)	20(10,10) - 20(9,11)	1v c	[79034]
	32482.72	(0.10)	18(8,10) - 18(7,11)	1v c	[79034]
	32498.42	(0.10)	16(6,10) - 16(5,11)	1v c	[79034]
	32509.59	(0.10)	14(4,10) - 14(3,11)	1v c	[79034]
	32517.21	(0.10)	12(2,10) - 12(1,11)	1v c	[79034]
	32520.00	(0.10)	11(1,10) - 11(0,11)	1v c	[79034]
	32593.45	(0.10)	6(3, 3) - 5(4, 2)	1v c	[79034]
	32755.70	(0.10)	6(4, 3) - 5(3, 2)	1v c	[79034]
	33198.40	(0.10)	7(2, 5) - 6(3, 4)	1v c	[79034]
	33736.39	(0.10)	8(1, 7) - 7(2, 6)	1v c	[79034]
	34275.15	(0.10)	9(1, 9) - 8(0, 8)	1v c	[79034]
	34753.00	(0.10)	6(4, 2) - 5(5, 1)	1v c	[79034]
	34887.03	(0.10)	5(5, 0) - 4(4, 1)	1v c	[79034]
	35388.45	(0.10)	30(19,11) - 30(18,12)	1v c	[79034]
	35443.00	(0.10)	28(17,11) - 28(16,12)	1v c	[79034]
	35487.40	(0.10)	26(15,11) - 26(14,12)	1v c	[79034]
	35522.90	(0.10)	24(13,11) - 24(12,12)	1v c	[79034]
	35551.20	(0.10)	22(11,11) - 22(10,12)	1v c	[79034]
	35573.06	(0.10)	20(9,11) - 20(8,12)	1v c	[79034]
	35602.17	(0.10)	16(5,11) - 16(4,12)	1v c	[79034]
	35611.08	(0.10)	14(3,11) - 14(2,12)	1v c	[79034]
	35617.29	(0.10)	12(1,11) - 12(0,12)	1v c	[79034]
	36295.00	(0.10)	7(3, 4) - 6(4, 3)	1v c	[79034]
	36306.16	(0.10)	7(4, 4) - 6(3, 3)	1v c	[79034]
	36479.50	(0.10)	6(5, 2) - 5(4, 1)	1v c	[79034]
	36834.21	(0.10)	8(2, 6) - 7(3, 5)	1v c	[79034]
	37372.48	(0.10)	9(2, 8) - 8(1, 7)	1v c	[79034]
	37636.18	(0.10)	5(4, 1) - 4(3, 2)	1v c	[79034]
	37911.32	(0.10)	10(1,10) - 9(0, 9)	1v c	[79034]
	38662.88	(0.10)	22(10,12) - 22(9,13)	1v c	[79034]
	38680.48	(0.10)	20(8,12) - 20(7,13)	1v c	[79034]
	38694.15	(0.10)	18(6,12) - 18(5,13)	1v c	[79034]
	38704.30	(0.10)	16(4,12) - 16(3,13)	1v c	[79034]
	38711.69	(0.10)	14(2,12) - 14(1,13)	1v c	[79034]
	38714.57	(0.10)	13(1,12) - 13(0,13)	1v c	[79034]
	39586.61	(0.10)	7(5, 3) - 6(4, 2)	1v c	[79034]
	39774.51	(0.10)	6(6, 1) - 5(5, 0)	1v c	[79034]

Table 77.1. Molecular constants of the ground state of Δ^6 -bicyclo[3.2.0]heptene.

Parameter	Normal [present]	$6\text{-}^{13}\text{C}$ [79035]
A'' (MHz)	4419.263(37)	4389.85
B'' (MHz)	3080.1918(74)	3033.45
C'' (MHz)	2375.3505(69)	2346.73
τ_1 (kHz)	-4.99(71)	
τ_2 (kHz)	-1.77(28)	
τ_3^a (kHz)	-32.3(237)	
τ_{aaaa} (kHz)	0 ^b	
τ_{bbbb} (kHz)	-0.89(45)	
τ_{cccc} (kHz)	-0.49(25)	
<u>Electric Dipole Moment</u> [79035]		
μ_a (D)	0.201(1)	
μ_c (D)	0.052(1)	

^aValue fixed by setting $R_6 = 0$.^bFixed at zero.Table 77.2. Molecular constants for the vibrational states of Δ^6 -bicyclo[3.2.0]heptene. [79035]

Vibrational state ^a (v_1, v_2, v_3)	A (MHz)	B (MHz)	C (MHz)
(0,0,0)	4419.20	3080.16	2375.33
(1,0,0)	4420.06	3078.47	2374.86
(0,1,0)	4424.16	3073.22	2369.70
(0,2,0)	4429.44	3066.49	2363.85
(0,1,1)	4427.19	3071.57	2366.83

^a v_1 is the twisting vibration of the five-membered ring, v_2 is the puckering vibration of the five-membered ring, and v_3 is the rocking of the four-membered ring.

TABLE 77.3. Microwave spectrum of bicyclo[3.2.0]hept-6-ene

C₇H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
CH(CHCH)CH ₂ CH ₂ CH ₂ CH	26806.75	(0.05)	5(2, 4) - 4(2, 3)		[79035]
	27678.27	(0.05)	5(3, 3) - 4(3, 2)		[79035]
<pre> HC = CH HC - CH H₂C CH₂ \ / CH₂ </pre>	27713.01	(0.05)	5(1, 4) - 4(1, 3)		[79035]
	27748.35	(0.05)	5(4, 2) - 4(4, 1)		[79035]
	27802.13	(0.05)	5(4, 1) - 4(4, 0)		[79035]
	28394.76	(0.05)	5(3, 2) - 4(3, 1)		[79035]
	29013.67	(0.05)	5(2, 3) - 4(2, 2)		[79035]
	29688.38	(0.05)	6(1, 6) - 5(1, 5)		[79035]
	29731.06	(0.05)	6(0, 6) - 5(0, 5)		[79035]
	31827.95	(0.05)	6(2, 5) - 5(2, 4)		[79035]
	32449.61	(0.05)	6(1, 5) - 5(1, 4)		[79035]
	33110.00	(0.05)	6(3, 4) - 5(3, 3)		[79035]
	33286.18	(0.05)	6(5, 2) - 5(5, 1)		[79035]
	33296.18	(0.05)	6(5, 1) - 5(5, 0)		[79035]
	33393.04	(0.05)	6(4, 3) - 5(4, 2)		[79035]
	33615.68	(0.05)	6(4, 2) - 5(4, 1)		[79035]
	34450.85	(0.05)	7(1, 7) - 6(1, 6)		[79035]
	34465.97	(0.05)	7(0, 7) - 6(0, 6)		[79035]
	34567.60	(0.05)	6(3, 3) - 5(3, 2)		[79035]
	34607.12	(0.05)	6(2, 4) - 5(2, 3)		[79035]
	36736.25	(0.05)	7(2, 6) - 6(2, 5)		[79035]
	37070.21	(0.05)	7(1, 6) - 6(1, 5)		[79035]
	38405.75	(0.05)	7(3, 5) - 6(3, 4)		[79035]
	38960.05	(0.05)	7(5, 3) - 6(5, 2)		[79035]
	39012.60	(0.05)	7(5, 2) - 6(5, 1)		[79035]
	39016.81	(0.05)	7(4, 4) - 6(4, 3)		[79035]
	39205.39	(0.05)	8(1, 8) - 7(1, 7)		[79035]
	39210.48	(0.05)	8(0, 8) - 7(0, 7)		[79035]
	39652.52	(0.05)	7(4, 3) - 6(4, 2)		[79035]
	39821.39	(0.05)	7(2, 5) - 6(2, 4)		[79035]
	27705.67	(0.05)	5(1, 4) - 4(1, 3)		1v tw [79035]
	26798.14	(0.05)	5(2, 4) - 4(2, 3)		1v tw [79035]
	28999.64	(0.05)	5(2, 3) - 4(2, 2)		1v tw [79035]
	27666.42	(0.05)	5(3, 3) - 4(3, 2)		1v tw [79035]
	28378.54	(0.05)	5(3, 2) - 4(3, 1)		1v tw [79035]
	27735.53	(0.05)	5(4, 2) - 4(4, 1)		1v tw [79035]
27788.66	(0.05)	5(4, 1) - 4(4, 0)		1v tw [79035]	
29724.88	(0.05)	6(0, 6) - 5(0, 5)		1v tw [79035]	
29682.00	(0.05)	6(1, 6) - 5(1, 5)		1v tw [79035]	
32442.87	(0.05)	6(1, 5) - 5(1, 4)		1v tw [79035]	
31818.73	(0.05)	6(2, 5) - 5(2, 4)		1v tw [79035]	
34593.07	(0.05)	6(2, 4) - 5(2, 3)		1v tw [79035]	
33096.67	(0.05)	6(3, 4) - 5(3, 3)		1v tw [79035]	
34547.30	(0.05)	6(3, 3) - 5(3, 2)		1v tw [79035]	
33377.39	(0.05)	6(4, 3) - 5(4, 2)		1v tw [79035]	
33597.93	(0.05)	6(4, 2) - 5(4, 1)		1v tw [79035]	
33270.55	(0.05)	6(5, 2) - 5(5, 1)		1v tw [79035]	
33280.57	(0.05)	6(5, 1) - 5(5, 0)		1v tw [79035]	
34458.90	(0.05)	7(0, 7) - 6(0, 6)		1v tw [79035]	
34443.40	(0.05)	7(1, 7) - 6(1, 6)		1v tw [79035]	
37063.01	(0.05)	7(1, 6) - 6(1, 5)		1v tw [79035]	
36726.57	(0.05)	7(2, 6) - 6(2, 5)		1v tw [79035]	
39809.32	(0.05)	7(2, 5) - 6(2, 4)		1v tw [79035]	
39391.89	(0.05)	7(3, 5) - 6(3, 4)		1v tw [79035]	
38999.00	(0.05)	7(4, 4) - 6(4, 3)		1v tw [79035]	
39629.19	(0.05)	7(4, 3) - 6(4, 2)		1v tw [79035]	
38941.73	(0.05)	7(5, 3) - 6(5, 2)		1v tw [79035]	
38993.25	(0.05)	7(5, 2) - 6(5, 1)		1v tw [79035]	
39202.45	(0.05)	8(0, 8) - 7(0, 7)		1v tw [79035]	
39197.25	(0.05)	8(1, 8) - 7(1, 7)		1v tw [79035]	
27661.63	(0.05)	5(1, 4) - 4(1, 3)		1v pu [79035]	
28946.96	(0.05)	5(2, 3) - 4(2, 2)		1v pu [79035]	
27613.59	(0.05)	5(3, 3) - 4(3, 2)		1v pu [79035]	
28319.60	(0.05)	5(3, 2) - 4(3, 1)		1v pu [79035]	
27680.90	(0.05)	5(4, 2) - 4(4, 1)		1v pu [79035]	
27733.33	(0.05)	5(4, 1) - 4(4, 0)		1v pu [79035]	
29666.20	(0.05)	6(0, 6) - 5(0, 5)		1v pu [79035]	

TABLE 77.3. Microwave spectrum of bicyclo[3.2.0]hept-6-ene — Continued

C₇H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J''(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	29622.30	(0.05)	6(1, 6) - 5(1, 5)	1v pu	[79035]
	32391.82	(0.05)	6(1, 5) - 5(1, 4)	1v pu	[79035]
	31760.65	(0.05)	6(2, 5) - 5(2, 4)	1v pu	[79035]
	34534.76	(0.05)	6(2, 4) - 5(2, 3)	1v pu	[79035]
	33034.86	(0.05)	6(3, 4) - 5(3, 3)	1v pu	[79035]
	34476.70	(0.05)	6(3, 3) - 5(3, 2)	1v pu	[79035]
	33312.04	(0.05)	6(4, 3) - 5(4, 2)	1v pu	[79035]
	33529.20	(0.05)	6(4, 2) - 5(4, 1)	1v pu	[79035]
	33205.00	(0.05)	6(5, 2) - 5(5, 1)	1v pu	[79035]
	33214.68	(0.05)	6(5, 1) - 5(5, 0)	1v pu	[79035]
	34389.81	(0.05)	7(0, 7) - 6(0, 6)	1v pu	[79035]
	34373.78	(0.05)	7(1, 7) - 6(1, 6)	1v pu	[79035]
	37001.80	(0.05)	7(1, 6) - 6(1, 5)	1v pu	[79035]
	36659.82	(0.05)	7(2, 6) - 6(2, 5)	1v pu	[79035]
	39747.38	(0.05)	7(2, 5) - 6(2, 4)	1v pu	[79035]
	38321.96	(0.05)	7(3, 5) - 6(3, 4)	1v pu	[79035]
	38923.64	(0.05)	7(4, 4) - 6(4, 3)	1v pu	[79035]
	38864.40	(0.05)	7(5, 3) - 6(5, 2)	1v pu	[79035]
	38915.15	(0.05)	7(5, 2) - 6(5, 1)	1v pu	[79035]
	39122.41	(0.05)	8(0, 8) - 7(0, 7)	1v pu	[79035]
	39117.19	(0.05)	8(1, 8) - 7(1, 7)	1v pu	[79035]

Table 78.1. Molecular constants of the axial and equatorial conformers of cyclopentyl acetylene.

Parameter	Equatorial [present]	Axial [present]
A'' (MHz)	6349.78(27)	4265.19(25)
B'' (MHz)	1765.1877(116)	2168.7636(95)
C'' (MHz)	1480.5470(132)	2032.0824(90)
τ_1 (kHz)	-6.230(210)	-11.89(33)
τ_2 (kHz)	-1.31(11)	-3.956(14)
τ_3^a (kHz)	-0.9(13.9)	182.(43.)
τ_{aaaa} (kHz)	0 ^b	0 ^b
τ_{bbbb} (kHz)	-0.432(221)	-2.73(29)
τ_{cccc} (kHz)	-0.23(24)	-4.46(26)
E (cm ⁻¹)	0 ^b	270 [83034]

^aValue fixed by setting R₆ = 0.^bFixed at zero.

TABLE 78.2. Microwave spectrum of cyclopentyl acetylene

C₇H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.	
<i>eq</i> -CH(CCH)CH ₂ CH ₂ CH ₂ CH ₂	28982.59	(0.10)	9(2, 8) - 8(2, 7)	[83034]	
	29253.98	(0.10)	9(8, 2) - 8(8, 1)	[83034]	
	29262.03	(0.10)	9(7, 3) - 8(7, 2)	[83034]	
	29274.43	(0.10)	9(6, 4) - 8(6, 3)	[83034]	
	29295.10	(0.10)	9(5, 5) - 8(5, 4)	[83034]	
	29331.55	(0.10)	9(4, 6) - 8(4, 5)	[83034]	
	29338.20	(0.10)	9(4, 5) - 8(4, 4)	[83034]	
	29349.72	(0.10)	9(3, 7) - 8(3, 6)	[83034]	
	29509.06	(0.10)	9(3, 6) - 8(3, 5)	[83034]	
	30180.66	(0.10)	9(2, 7) - 8(2, 6)	[83034]	
	30645.72	(0.10)	10(1, 10) - 9(1, 9)	[83034]	
	32137.83	(0.10)	10(2, 9) - 9(2, 8)	[83034]	
	32503.17	(0.10)	10(9, 2) - 9(9, 1)	[83034]	
	32510.78	(0.10)	10(8, 3) - 9(8, 2)	[83034]	
	32521.80	(0.10)	10(7, 4) - 9(7, 3)	[83034]	
	32538.74	(0.10)	10(6, 5) - 9(6, 4)	[83034]	
	32567.03	(0.10)	10(5, 6) - 9(5, 5)	[83034]	
	32614.79	(0.10)	10(4, 7) - 9(4, 6)	[83034]	
	32619.77	(0.10)	10(3, 8) - 9(3, 7)	[83034]	
	32629.01	(0.10)	10(4, 6) - 9(4, 5)	[83034]	
	32885.25	(0.10)	10(3, 7) - 9(3, 6)	[83034]	
	33226.17	(0.10)	10(1, 9) - 9(1, 8)	[83034]	
	33636.76	(0.10)	10(2, 8) - 9(2, 7)	[83034]	
	33645.62	(0.10)	11(1, 11) - 10(1, 10)	[83034]	
	35274.22	(0.10)	11(2, 10) - 10(2, 9)	[83034]	
	35752.22	(0.10)	11(10, 2) - 10(10, 1)	[83034]	
	35759.55	(0.10)	11(9, 3) - 10(9, 2)	[83034]	
	35769.68	(0.10)	11(8, 4) - 10(8, 3)	[83034]	
	35784.24	(0.10)	11(7, 5) - 10(7, 4)	[83034]	
	35806.74	(0.10)	11(6, 6) - 10(6, 5)	[83034]	
	35844.30	(0.10)	11(5, 7) - 10(5, 6)	[83034]	
	35844.98	(0.10)	11(5, 6) - 10(5, 5)	[83034]	
	35884.36	(0.10)	11(3, 9) - 10(3, 8)	[83034]	
	35904.01	(0.10)	11(4, 8) - 10(4, 7)	[83034]	
	35932.03	(0.10)	11(4, 7) - 10(4, 6)	[83034]	
	36299.00	(0.10)	11(3, 8) - 10(3, 7)	[83034]	
	36360.98	(0.10)	11(1, 10) - 10(1, 9)	[83034]	
	37073.04	(0.10)	11(2, 9) - 10(2, 8)	[83034]	
	<i>ax</i> -CH(CCH)CH ₂ CH ₂ CH ₂ CH ₂	28852.54	(0.10)	7(1, 7) - 6(1, 6)	[83034]
		29081.78	(0.10)	7(0, 7) - 6(0, 6)	[83034]
		29354.49	(0.10)	7(2, 6) - 6(2, 5)	[83034]
		29446.94	(0.10)	7(3, 5) - 6(3, 4)	[83034]
		29470.75	(0.10)	7(3, 4) - 6(3, 3)	[83034]
		29676.78	(0.10)	7(2, 5) - 6(2, 4)	[83034]
		29785.91	(0.10)	7(1, 6) - 6(1, 5)	[83034]
		32950.76	(0.10)	8(1, 8) - 7(1, 7)	[83034]
		33151.96	(0.10)	8(0, 8) - 7(0, 7)	[83034]
33526.24		(0.10)	8(2, 7) - 7(2, 6)	[83034]	
33629.17		(0.10)	8(6, 3) - 7(6, 2)	[83034]	
33649.66		(0.10)	8(4, 5) - 7(4, 4)	[83034]	
33651.26		(0.10)	8(4, 4) - 7(4, 3)	[83034]	
33660.25		(0.10)	8(3, 6) - 7(3, 5)	[83034]	
33706.80		(0.10)	8(3, 5) - 7(3, 4)	[83034]	
33977.69		(0.10)	8(2, 6) - 7(2, 5)	[83034]	
33997.92		(0.10)	8(1, 7) - 7(1, 6)	[83034]	
37042.37		(0.10)	9(1, 9) - 8(1, 8)	[83034]	
37209.11		(0.10)	9(0, 9) - 8(0, 8)	[83034]	
37689.82		(0.10)	9(2, 8) - 8(2, 7)	[83034]	
37826.91		(0.10)	9(8, 1) - 8(8, 0)	[83034]	
37830.90		(0.10)	9(7, 3) - 8(7, 2)	[83034]	
37837.00		(0.10)	9(6, 4) - 8(6, 3)	[83034]	
37847.40		(0.10)	9(5, 5) - 8(5, 4)	[83034]	
37865.45		(0.10)	9(4, 6) - 8(4, 5)	[83034]	
37869.11		(0.10)	9(4, 5) - 8(4, 4)	[83034]	
37873.08		(0.10)	9(3, 7) - 8(3, 6)	[83034]	
37956.86		(0.10)	9(3, 6) - 8(3, 5)	[83034]	
38189.26		(0.10)	9(1, 8) - 8(1, 7)	[83034]	
38281.95		(0.10)	9(2, 7) - 8(2, 6)	[83034]	

Table 79.1. Molecular constants of bicyclo[2.2.1]heptane (norbornane).

Parameter	Value	Reference
A (MHz)	3694.2465(46)	[present]
B (MHz)	3212.5660(30)	[present]
C (MHz)	2775.813(18)	[present]
μ_c (D)	0.091(8)	[80034]

TABLE 79.2. Microwave spectrum of bicyclo[2.2.1] heptane

C₇H₁₂


Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
$\text{CH}(\text{CH}_2)\text{CH}_2\text{CH}_2\text{CHCH}_2\text{CH}$ 	26908.89	(0.10)	4(1, 3) - 3(0, 3)	[80034]
	27310.19	(0.10)	4(2, 3) - 3(1, 3)	[80034]
	27822.02	(0.10)	4(3, 2) - 3(2, 2)	[80034]
	33305.67	(0.10)	5(2, 3) - 4(1, 3)	[80034]
	33478.47	(0.10)	5(3, 2) - 4(2, 2)	[80034]
	33854.15	(0.10)	5(1, 4) - 4(0, 4)	[80034]
	34021.08	(0.10)	5(2, 4) - 4(1, 4)	[80034]
	34237.00	(0.10)	5(3, 3) - 4(2, 3)	[80034]
	35047.05	(0.10)	5(4, 2) - 4(3, 2)	[80034]
	39857.43	(0.10)	6(3, 3) - 5(2, 3)	[80034]

Table 80.1. Molecular constants for methylene cyclohexane. [84026]

Vibrational state ^a (v_1, v_2)	A (MHz)	B (MHz)	C (MHz)
(0,0)	4090.85(1)	2482.13(1)	1749.49(1)
(1,0)	4083.23(13)	2484.20(1)	1751.09(1)
(2,0)	4075.99(9)	2486.16(1)	1752.58(1)
(3,0)	4068.28(12)	2488.01(1)	1753.97(1)
(4,0)	4062.28(12)	2489.76(1)	1755.25(1)
(0,1)	4094.79(10)	2480.81(1)	1749.00(1)

Electric Dipole Moment

$$(0,0) \mu_a = 0.61(1) \text{ D}$$

$$\mu_b = 0 \text{ (assumed)}$$

$$\mu_c = 0.11(1) \text{ D}$$

^aThe ring bending vibration is v_1 and ring twisting vibration is v_2 .

TABLE 80.2. Microwave spectrum of methylene cyclohexane

C₇H₁₂

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
CH ₂ (CH ₂) ₄ CCH ₂	18731.03	(0.05)	5(1, 5) - 4(1, 4)	1v t	[84026]
	18736.07	(0.05)	5(1, 5) - 4(1, 4)		[84026]
	18750.90	(0.05)	5(1, 5) - 4(1, 4)	1v b	[84026]
	18764.68	(0.05)	5(1, 5) - 4(1, 4)	2v b	[84026]
	18777.46	(0.05)	5(1, 5) - 4(1, 4)	3v b	[84026]
	18789.28	(0.05)	5(1, 5) - 4(1, 4)	4v b	[84026]
	18888.70	(0.05)	5(0, 5) - 4(0, 4)	1v t	[84026]
	18892.46	(0.05)	5(0, 5) - 4(0, 4)		[84026]
	18905.27	(0.05)	5(0, 5) - 4(0, 4)	1v b	[84026]
	18917.10	(0.05)	5(0, 5) - 4(0, 4)	2v b	[84026]
	18928.04	(0.05)	5(0, 5) - 4(0, 4)	3v b	[84026]
	18938.11	(0.05)	5(0, 5) - 4(0, 4)	4v b	[84026]
	20712.07	(0.05)	5(2, 4) - 4(2, 3)	1v t	[84026]
	20719.16	(0.05)	5(2, 4) - 4(2, 3)		[84026]
	20735.01	(0.05)	5(2, 4) - 4(2, 3)	1v b	[84026]
	20749.75	(0.05)	5(2, 4) - 4(2, 3)	2v b	[84026]
	20763.63	(0.05)	5(2, 4) - 4(2, 3)	3v b	[84026]
	20776.38	(0.05)	5(2, 4) - 4(2, 3)	4v b	[84026]
	21773.03	(0.05)	5(1, 4) - 4(1, 3)	1v t	[84026]
	21777.87	(0.05)	5(1, 4) - 4(1, 3)		[84026]
	21789.19	(0.05)	5(1, 4) - 4(1, 3)	1v b	[84026]
	21799.64	(0.05)	5(1, 4) - 4(1, 3)	2v b	[84026]
	21809.18	(0.05)	5(1, 4) - 4(1, 3)	3v b	[84026]
	21817.88	(0.05)	5(1, 4) - 4(1, 3)	4v b	[84026]
	22271.96	(0.05)	6(1, 6) - 5(1, 5)	1v t	[84026]
	22277.63	(0.05)	6(1, 6) - 5(1, 5)		[84026]
	22295.22	(0.05)	6(1, 6) - 5(1, 5)	1v b	[84026]
	22311.55	(0.05)	6(1, 6) - 5(1, 5)	2v b	[84026]
	22326.61	(0.05)	6(1, 6) - 5(1, 5)	3v b	[84026]
	22340.60	(0.05)	6(1, 6) - 5(1, 5)	4v b	[84026]
	22338.94	(0.05)	6(0, 6) - 5(0, 5)	1v t	[84026]
	22343.94	(0.05)	6(0, 6) - 5(0, 5)		[84026]
	22360.37	(0.05)	6(0, 6) - 5(0, 5)	1v b	[84026]
	22375.62	(0.05)	6(0, 6) - 5(0, 5)	2v b	[84026]
	22389.70	(0.05)	6(0, 6) - 5(0, 5)	3v b	[84026]
	22402.69	(0.05)	6(0, 6) - 5(0, 5)	4v b	[84026]
	22517.61	(0.05)	3(3, 0) - 2(2, 0)		[84026]
	22681.18	(0.05)	3(3, 1) - 2(2, 1)		[84026]
	22817.62	(0.05)	4(1, 3) - 3(0, 3)		[84026]
	22933.05	(0.05)	5(2, 3) - 4(2, 2)	1v t	[84026]
	22944.97	(0.05)	5(2, 3) - 4(2, 2)		[84026]
	22965.68	(0.05)	5(2, 3) - 4(2, 2)	1v b	[84026]
22985.24	(0.05)	5(2, 3) - 4(2, 2)	2v b	[84026]	
23003.64	(0.05)	5(2, 3) - 4(2, 2)	3v b	[84026]	
23013.54	(0.05)	4(2, 2) - 3(1, 2)		[84026]	
23020.90	(0.05)	5(2, 3) - 4(2, 2)	4v b	[84026]	
24530.36	(0.05)	6(2, 5) - 5(2, 4)	1v t	[84026]	
24537.66	(0.05)	6(2, 5) - 5(2, 4)		[84026]	
24555.13	(0.05)	6(2, 5) - 5(2, 4)	1v b	[84026]	
24571.40	(0.05)	6(2, 5) - 5(2, 4)	2v b	[84026]	
24586.41	(0.05)	6(2, 5) - 5(2, 4)	3v b	[84026]	
24600.47	(0.05)	6(2, 5) - 5(2, 4)	4v b	[84026]	
25003.19	(0.05)	4(2, 3) - 3(1, 3)		[84026]	
25335.97	(0.05)	6(1, 5) - 5(1, 4)	1v t	[84026]	
25339.30	(0.05)	6(1, 5) - 5(1, 4)		[84026]	
25349.91	(0.05)	6(1, 5) - 5(1, 4)	1v b	[84026]	
25359.64	(0.05)	6(1, 5) - 5(1, 4)	2v b	[84026]	
25368.38	(0.05)	6(1, 5) - 5(1, 4)	3v b	[84026]	
25376.28	(0.05)	6(1, 5) - 5(1, 4)	4v b	[84026]	
26548.78	(0.05)	4(3, 1) - 3(2, 1)		[84026]	

Table 81.1. Molecular constants of phenylacetylene.

Parameter	C_6H_5CCH
A" (MHz)	5680.692(132)
B" (MHz)	1529.7460(80)
C" (MHz)	1204.9589(92)
τ_1 (kHz)	4.370(64)
τ_2 (kHz)	0.8822(35)
τ_3^a (kHz)	6.8(26)
τ_{aaaa} (kHz)	0 ^b
τ_{bbbb} (kHz)	-0.125(98)
τ_{cccc} (kHz)	-0.180(122)
<u>Electric Dipole Moment</u> [75054]	
μ_a (D)	0.656(5)

^aValue fixed by setting $R_6 = 0$.

^bFixed at zero.

Table 81.2. Molecular constants for some isotopically substituted species of phenylacetylene.

Species	A (MHz)	B (MHz)	C (MHz)
$C_6H_5CCD^a$	5680.8(6)	1450.244(4)	1155.061(4)
2- ¹³ C	(5589.4) ^b	B+C = 2730.442(5)	
3- ¹³ C	5589.3(20)	1518.985(15)	1194.185(15)
4- ¹³ C	(5680.3) ^b	1507.181(10)	1190.910(10)
7- ¹³ C	(5680.3) ^b	1511.566(10)	1193.646(10)
8- ¹³ C	(5680.3) ^b	1483.818(10)	1176.276(10)

^aFor this species $D_J=0.023(3)$ kHz and $D_{JK}=1.07(1)$ kHz were determined.

^bAssumed values.

TABLE 81.3. Microwave spectrum of phenylacetylene

C₂H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$	-	$J''(K_{-1}, K_{+1})$	Ref.
C(CCH)CHCHCHCHCH	21933.80	(0.50)	8(7, 1)	-	7(7, 0)	[60008]
	21945.90	(0.50)	8(6, 2)	-	7(6, 1)	[60008]
	21966.70	(0.50)	8(5, 3)	-	7(5, 2)	[60008]
	22003.40	(0.50)	8(4, 5)	-	7(4, 4)	[60008]
	22009.50	(0.50)	8(4, 4)	-	7(4, 3)	[60008]
	22023.45	(0.05)	8(3, 6)	-	7(3, 5)	[75054]
	22178.73	(0.05)	8(3, 5)	-	7(3, 4)	[75054]
	24674.50	(0.50)	9(8, 1)	-	8(8, 0)	[60008]
	24685.60	(0.50)	9(7, 2)	-	8(7, 1)	[60008]
	24702.75	(0.05)	9(6, 4)	-	8(6, 3)	[75054]
	24732.10	(0.50)	9(5, 5)	-	8(5, 4)	[60008]
	24796.40	(0.50)	9(4, 5)	-	8(4, 4)	[60008]
	30079.87	(0.05)	12(1,12)	-	11(1,11)	[75054]
	30191.21	(0.05)	12(0,12)	-	11(0,11)	[75054]
	32037.04	(0.05)	12(2,11)	-	11(2,10)	[75054]
	32581.63	(0.05)	13(0,13)	-	12(0,12)	[75054]
	32893.84	(0.05)	12(11, 1)	-	11(11, 0)	[75054]
	32903.73	(0.05)	12(10, 2)	-	11(10, 1)	[75054]
	32916.89	(0.05)	12(9, 3)	-	11(9, 2)	[75054]
	32935.18	(0.05)	12(8, 4)	-	11(8, 3)	[75054]
	32961.85	(0.05)	12(7, 5)	-	11(7, 4)	[75054]
	32988.31	(0.05)	12(1,11)	-	11(1,10)	[75054]
	33003.35	(0.05)	12(6, 6)	-	11(6, 5)	[75054]
	33017.26	(0.05)	12(3,10)	-	11(3, 9)	[75054]
	33071.33	(0.05)	12(5, 8)	-	11(5, 7)	[75054]
	33076.94	(0.05)	12(5, 7)	-	11(5, 6)	[75054]
	33157.59	(0.05)	12(4, 9)	-	11(4, 8)	[75054]
	33270.59	(0.05)	12(4, 8)	-	11(4, 7)	[75054]
	34000.93	(0.05)	12(3, 9)	-	11(3, 8)	[75054]
	34548.74	(0.05)	12(2,10)	-	11(2, 9)	[75054]
	34570.51	(0.05)	13(2,12)	-	12(2,11)	[75054]
	35391.29	(0.05)	13(1,12)	-	12(1,11)	[75054]
	35633.62	(0.05)	13(12, 2)	-	12(12, 1)	[75054]
	35643.22	(0.05)	13(11, 3)	-	12(11, 2)	[75054]
	35655.70	(0.05)	13(10, 4)	-	12(10, 3)	[75054]
	35672.33	(0.05)	13(9, 5)	-	12(9, 4)	[75054]
	35695.51	(0.05)	13(8, 6)	-	12(8, 5)	[75054]
	35726.43	(0.05)	13(3,11)	-	12(3,10)	[75054]
	35729.41	(0.05)	13(7, 7)	-	12(7, 6)	[75054]
	35782.40	(0.05)	13(6, 8)	-	12(6, 7)	[75054]
	35867.16	(0.05)	13(5, 9)	-	12(5, 8)	[75054]
	35878.85	(0.05)	13(5, 8)	-	12(5, 7)	[75054]
	35957.27	(0.05)	13(4,10)	-	12(4, 9)	[75054]
	36151.92	(0.05)	13(4, 9)	-	12(4, 8)	[75054]
	37051.51	(0.05)	13(3,10)	-	12(3, 9)	[75054]
	37344.62	(0.05)	13(2,11)	-	12(2,10)	[75054]
	38373.20	(0.05)	14(13, 1)	-	13(13, 0)	[75054]
38382.66	(0.05)	14(12, 2)	-	13(12, 1)	[75054]	
38394.55	(0.05)	14(11, 3)	-	13(11, 2)	[75054]	
38410.05	(0.05)	14(10, 4)	-	13(10, 3)	[75054]	
38412.36	(0.05)	14(3,12)	-	13(3,11)	[75054]	
38430.79	(0.05)	14(9, 5)	-	13(9, 4)	[75054]	
38459.69	(0.05)	14(8, 7)	-	13(8, 6)	[75054]	
38502.06	(0.05)	14(7, 8)	-	13(7, 7)	[75054]	
38568.49	(0.05)	14(6, 9)	-	13(6, 8)	[75054]	
38671.27	(0.05)	14(5,10)	-	13(5, 9)	[75054]	
38694.21	(0.05)	14(5, 9)	-	13(5, 8)	[75054]	
38755.81	(0.05)	14(4,11)	-	13(4,10)	[75054]	
39073.19	(0.05)	14(4,10)	-	13(4, 9)	[75054]	
C(CCH) ¹³ CHCHCHCHCH	38317.90	(0.15)	14(13, 1)	-	13(13, 0)	[75054]
	38327.83	(0.15)	14(12, 2)	-	13(12, 1)	[75054]
	38340.43	(0.15)	14(11, 3)	-	13(11, 2)	[75054]
	38356.54	(0.15)	14(10, 4)	-	13(10, 3)	[75054]
	35592.75	(0.15)	13(11, 2)	-	12(11, 1)	[75054]
	35605.56	(0.15)	13(10, 3)	-	12(10, 2)	[75054]
	35622.83	(0.15)	13(9, 4)	-	12(9, 3)	[75054]
C(CCH)CH ¹³ CHCHCHCH	38095.48	(0.15)	14(11, 3)	-	13(11, 2)	[75054]
	38111.20	(0.15)	14(10, 4)	-	13(10, 3)	[75054]

TABLE 81.3. Microwave spectrum of phenylacetylene — Continued

C₈H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
	38132.41	(0.15)	14(9, 5) - 13(9, 4)	[75054]
	38161.74	(0.15)	14(8, 6) - 13(8, 5)	[75054]
	38204.87	(0.15)	14(7, 7) - 13(7, 6)	[75054]
	38272.52	(0.15)	14(6, 8) - 13(6, 7)	[75054]
	35394.92	(0.15)	13(9, 4) - 12(9, 3)	[75054]
	35418.56	(0.15)	13(8, 5) - 12(8, 4)	[75054]
	35452.92	(0.15)	13(7, 6) - 12(7, 5)	[75054]
	35507.02	(0.15)	13(6, 7) - 12(6, 6)	[75054]
	35592.86	(0.15)	13(5, 9) - 12(5, 8)	[75054]
	35605.57	(0.15)	13(5, 8) - 12(5, 7)	[75054]
C(CCH)CHCH ¹³ CHCHCH	37890.69	(0.15)	14(10, 4) - 13(10, 3)	[75054]
	37910.03	(0.15)	14(9, 5) - 13(9, 4)	[75054]
	37937.53	(0.15)	14(8, 6) - 13(8, 5)	[75054]
	37977.29	(0.15)	14(7, 7) - 13(7, 6)	[75054]
	38040.17	(0.15)	14(6, 8) - 13(6, 7)	[75054]
	38157.80	(0.15)	14(5, 9) - 13(5, 8)	[75054]
	35211.51	(0.15)	13(8, 5) - 12(8, 4)	[75054]
	35293.50	(0.15)	13(6, 6) - 12(6, 5)	[75054]
C(¹³ CCH)CHCHCHCHCH	38039.09	(0.15)	14(8, 6) - 13(8, 5)	[75054]
	38079.55	(0.15)	14(7, 7) - 13(7, 6)	[75054]
	38142.87	(0.15)	14(6, 8) - 13(6, 7)	[75054]
	38241.44	(0.15)	14(5,10) - 13(5, 9)	[75054]
	35305.64	(0.15)	13(8, 5) - 12(8, 4)	[75054]
	35388.61	(0.15)	13(6, 7) - 12(6, 6)	[75054]
	32575.81	(0.15)	12(8, 5) - 11(8, 4)	[75054]
C(C ¹³ CH)CHCHCHCHCH	37370.05	(0.15)	14(9, 5) - 13(9, 4)	[75054]
	37395.75	(0.15)	14(8, 6) - 13(8, 5)	[75054]
	37492.24	(0.15)	14(6, 8) - 13(6, 7)	[75054]
	37585.11	(0.15)	14(5,10) - 13(5, 9)	[75054]
	34709.43	(0.15)	13(8, 5) - 12(8, 4)	[75054]
	34786.60	(0.15)	13(6, 7) - 12(6, 6)	[75054]
C(CCD)CHCHCHCHCH	36615.42	(0.05)	14(8, 7) - 13(8, 6)	[75054]
	33935.32	(0.05)	13(12, 2) - 12(12, 1)	[75054]
	33943.29	(0.05)	13(11, 3) - 12(11, 2)	[75054]
	33953.57	(0.05)	13(10, 4) - 12(10, 3)	[75054]
	33967.21	(0.05)	13(9, 5) - 12(9, 4)	[75054]
	33986.16	(0.05)	13(8, 6) - 12(8, 5)	[75054]
	34013.78	(0.05)	13(7, 7) - 12(7, 6)	[75054]
	34056.88	(0.05)	13(6, 8) - 12(6, 7)	[75054]
	34126.80	(0.05)	13(5, 9) - 12(5, 8)	[75054]
	34133.61	(0.05)	13(5, 8) - 12(5, 7)	[75054]
	34211.12	(0.05)	13(4,10) - 12(4, 9)	[75054]
	34340.92	(0.05)	13(4, 9) - 12(4, 8)	[75054]
	33059.63	(0.05)	13(2,12) - 12(2,11)	[75054]
	35552.81	(0.05)	13(2,11) - 12(2,10)	[75054]
	31334.21	(0.05)	12(10, 2) - 11(10, 1)	[75054]
	31344.97	(0.05)	12(9, 3) - 11(9, 2)	[75054]
	31360.01	(0.05)	12(8, 4) - 11(8, 3)	[75054]
	31381.73	(0.05)	12(7, 5) - 11(7, 4)	[75054]
	31415.56	(0.05)	12(6, 6) - 11(6, 5)	[75054]
	31548.29	(0.05)	12(4, 9) - 11(4, 8)	[75054]
	31623.22	(0.05)	12(4, 8) - 11(4, 7)	[75054]
	30622.64	(0.05)	12(2,11) - 11(2,10)	[75054]
	32854.42	(0.05)	12(2,10) - 11(2, 9)	[75054]
	23521.24	(0.05)	9(6, 4) - 8(6, 3)	[75054]

Table 82.1. Molecular constants of methylene cycloheptatriene (heptafulvene).

Species	A (MHz)	B (MHz)	C (MHz)	Reference
<u>Rotational Constants</u>				
Ground State	3666.011(155)	2004.2877(153)	1297.501(181)	[present]
$\nu_{4_2} = 1$	3654.53(59)	2008.489(56)	1302.525(99)	[76055]
$\nu_{4_2} = 2$	3640.46(95)	2012.436(96)	1307.64(10)	[76055]
$\nu_{4_2} = 3$	3620.9(1.3)	2015.72(25)	1313.47(27)	[76055]
$\nu_{4_2} = 4$	3617.9(2.4)	2020.74(26)	1317.34(29)	[76055]
<u>Electric Dipole Moment</u> [76055]				
μ_a	0.4765(50) D			

TABLE 82.2. Microwave spectrum of methylene cycloheptatriene

C₇H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
C(CH ₂)CHCHCHCHCHCH	26997.75	(0.05)	8(7, 2) - 7(7, 1)		[76055]
	27121.35	(0.05)	8(6, 3) - 7(6, 2)		[76055]
	27125.91	(0.05)	8(6, 2) - 7(6, 1)		[76055]
	27303.05	(0.05)	8(4, 5) - 7(4, 4)		[76055]
	28261.98	(0.05)	8(4, 4) - 7(4, 3)		[76055]
	30358.90	(0.05)	9(8, 2) - 8(8, 1)		[76055]
	30473.17	(0.05)	9(7, 3) - 8(7, 2)		[76055]
	30473.57	(0.05)	9(7, 2) - 8(7, 1)		[76055]
	30651.91	(0.05)	9(4, 6) - 8(4, 5)		[76055]
	30839.76	(0.05)	9(5, 5) - 8(5, 4)		[76055]
	31139.00	(0.05)	9(5, 4) - 8(5, 3)		[76055]
	32404.76	(0.05)	9(4, 5) - 8(4, 4)		[76055]
	33720.78	(0.05)	10(9, 2) - 9(9, 1)		[76055]
	33827.18	(0.05)	10(8, 3) - 9(8, 2)		[76055]
	33874.78	(0.05)	10(4, 7) - 9(4, 6)		[76055]
	33984.48	(0.05)	10(7, 4) - 9(7, 3)		[76055]
	33987.93	(0.05)	10(7, 3) - 9(7, 2)		[76055]
	34210.08	(0.05)	10(6, 5) - 9(6, 4)		[76055]
	34281.14	(0.05)	10(6, 4) - 9(6, 3)		[76055]
	34367.29	(0.05)	10(5, 6) - 9(5, 5)		[76055]
	35086.67	(0.05)	10(5, 5) - 9(5, 4)		[76055]
	36504.90	(0.05)	10(4, 6) - 9(4, 5)		[76055]
	37083.16	(0.05)	11(10, 2) - 10(10, 1)		[76055]
	37183.66	(0.05)	11(9, 3) - 10(9, 2)		[76055]
	37326.53	(0.05)	11(8, 4) - 10(8, 3)		[76055]
	37326.87	(0.05)	11(8, 3) - 10(8, 2)		[76055]
	37535.81	(0.05)	11(7, 5) - 10(7, 4)		[76055]
	37550.12	(0.05)	11(7, 4) - 10(7, 3)		[76055]
	37802.09	(0.05)	11(6, 6) - 10(6, 5)		[76055]
	37832.93	(0.05)	11(5, 7) - 10(5, 6)		[76055]
	38009.38	(0.05)	11(6, 5) - 10(6, 4)		[76055]
	39257.39	(0.05)	11(5, 6) - 10(5, 5)		[76055]
	27199.25	(0.05)	8(6, 3) - 7(6, 2)	1v ₄₂	[76055]
	27203.86	(0.05)	8(6, 2) - 7(6, 1)	1v ₄₂	[76055]
	30445.51	(0.05)	9(8, 2) - 8(8, 1)	1v ₄₂	[76055]
	34308.77	(0.05)	10(6, 5) - 9(6, 4)	1v ₄₂	[76055]
	35197.46	(0.05)	10(5, 5) - 9(5, 4)	1v ₄₂	[76055]
	36607.11	(0.05)	10(4, 6) - 9(4, 5)	1v ₄₂	[76055]
	37188.92	(0.05)	11(10, 2) - 10(10, 1)	1v ₄₂	[76055]
	37290.09	(0.05)	11(9, 3) - 10(9, 2)	1v ₄₂	[76055]
	37644.39	(0.05)	11(7, 5) - 10(7, 4)	1v ₄₂	[76055]
	37659.20	(0.05)	11(7, 4) - 10(7, 3)	1v ₄₂	[76055]
	37910.62	(0.05)	11(6, 6) - 10(6, 5)	1v ₄₂	[76055]
	37934.70	(0.05)	11(5, 7) - 10(5, 6)	1v ₄₂	[76055]
	38124.36	(0.05)	11(6, 5) - 10(6, 4)	1v ₄₂	[76055]
	39384.39	(0.05)	11(5, 6) - 10(5, 5)	1v ₄₂	[76055]
	37293.7	(0.1)	11(10, 2) - 10(10, 1)	2v ₄₂	[76055]
	37395.3	(0.1)	11(9, 3) - 10(9, 2)	2v ₄₂	[76055]
	37540.0	(0.1)	11(8, 4) - 10(8, 3)	2v ₄₂	[76055]
	37540.5	(0.1)	11(8, 3) - 10(8, 2)	2v ₄₂	[76055]
	37751.5	(0.1)	11(7, 5) - 10(7, 4)	2v ₄₂	[76055]
	38017.8	(0.1)	11(6, 6) - 10(6, 5)	2v ₄₂	[76055]
	38238.3	(0.1)	11(6, 5) - 10(6, 4)	2v ₄₂	[76055]
	37397.9	(0.1)	11(10, 2) - 10(10, 1)	3v ₄₂	[76055]
	37500.0	(0.1)	11(9, 3) - 10(9, 2)	3v ₄₂	[76055]
	37645.4	(0.1)	11(8, 4) - 10(8, 3)	3v ₄₂	[76055]
	37646.1	(0.1)	11(8, 3) - 10(8, 2)	3v ₄₂	[76055]
	37874.5	(0.1)	11(7, 4) - 10(7, 3)	3v ₄₂	[76055]
	38351.8	(0.1)	11(6, 5) - 10(6, 4)	3v ₄₂	[76055]
	37604.3	(0.1)	11(9, 3) - 10(9, 2)	4v ₄₂	[76055]
	37965.0	(0.1)	11(7, 5) - 10(7, 4)	4v ₄₂	[76055]
	37981.6	(0.1)	11(7, 4) - 10(7, 3)	4v ₄₂	[76055]
	38465.1	(0.1)	11(6, 5) - 10(6, 4)	4v ₄₂	[76055]

Table 83.1. Rotational constants for o-xylene. [73086]

o-Xylene Species	A (MHz)	B (MHz)	C (MHz)	V_3 (cm^{-1})
<u>Rotational Constants</u>				
$\text{CH}_3\text{C}_6\text{H}_4\text{CH}_3$	3163.930(50)	2150.069(5)	1300.835(5)	519.(3)
sym- $\text{CH}_2\text{DC}_6\text{H}_4\text{CH}_3$	3045.778(100)	2123.611(10)	1271.100(10)	528.(9)
asy- $\text{CDH}_2\text{C}_6\text{H}_4\text{CH}_3$	3123.019(100)	2089.736(10)	1276.442(10)	521.(8)
sym- $\text{CD}_2\text{HC}_6\text{H}_4\text{CH}_3$	3085.147(100)	2032.070(10)	1253.577(10)	527.(8)
asy- $\text{CHD}_2\text{C}_6\text{H}_4\text{CH}_3$	3014.161(100)	2062.862(10)	1248.191(10)	474.(13)
$\text{CD}_3\text{C}_6\text{H}_4\text{CH}_3$	2984.204(100)	2005.184(10)	1226.690(10)	560.(24)
$^{13}\text{CH}_3\text{C}_6\text{H}_4\text{CH}_3$	3123.542(50)	2119.462(5)	1282.807(5)	518.(6)
$3d_1\text{-CH}_3\text{C}_6\text{DH}_3\text{CH}_3$	3048.552(50)	2145.490(10)	1279.293(5)	518.(11)
$4d_1\text{-CH}_3\text{C}_6\text{H}_3\text{DCH}_3$	3136.641(100)	2077.688(10)	1269.542(10)	527.(21)
				$V_3(\text{ave}) = 521.(17)$
<u>Electric Dipole Moment (normal species)</u>				
μ_a (D)	0.640(5)			

TABLE 83.2. Microwave spectrum of ortho-xylene

C₈H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$	-	$J''(K_{-1}, K_{+1})$	Sym.	Ref.
C(CH ₃)(CH) ₂ CCH ₃	9214.140	(0.030)	3(0, 3)	-	2(0, 2)		[73086]
	10898.76	(0.05)	49(24,25)	-	49(24,26)	AA	[73086]
	10901.46	(0.05)	49(24,25)	-	49(24,26)	EE	[73086]
	10903.84	(0.05)	49(24,25)	-	49(24,26)	EA	[73086]
	10904.38	(0.05)	49(24,25)	-	49(24,26)	AE	[73086]
	11198.00	(0.05)	47(23,25)	-	47(23,24)	AA	[73086]
	11200.59	(0.05)	47(23,25)	-	47(23,24)	EE	[73086]
	11202.97	(0.05)	47(23,25)	-	47(23,24)	EA	[73086]
	11203.47	(0.05)	47(23,25)	-	47(23,24)	AE	[73086]
	11334.277	(0.030)	3(1, 2)	-	2(1, 1)		[73086]
	11477.79	(0.05)	45(22,23)	-	45(22,24)	AA	[73086]
	11480.34	(0.05)	45(22,23)	-	45(22,24)	AA	[73086]
	11482.64	(0.05)	45(22,23)	-	45(22,24)	EA	[73086]
	11483.10	(0.05)	45(22,23)	-	45(22,24)	AE	[73086]
	11548.57	(0.05)	19(9,10)	-	19(9,11)	AA	[73086]
	11549.26	(0.05)	19(9,10)	-	19(9,11)	EE	[73086]
	11549.90	(0.05)	19(9,10)	-	19(9,11)	EA+AE	[73086]
	11604.253	(0.030)	4(1, 4)	-	3(1, 3)		[73086]
	11734.69	(0.05)	43(21,22)	-	43(21,23)	AA	[73086]
	11737.14	(0.05)	43(21,22)	-	43(21,23)	EE	[73086]
	11738.564	(0.030)	4(0, 4)	-	3(0, 3)		[73086]
	11739.39	(0.05)	43(21,22)	-	43(21,23)	EA	[73086]
	11739.80	(0.05)	43(21,22)	-	43(21,23)	AE	[73086]
	11894.54	(0.05)	21(10,11)	-	21(10,12)	AA	[73086]
	11895.35	(0.05)	21(10,11)	-	21(10,12)	EE	[73086]
	11896.13	(0.05)	21(10,11)	-	21(10,12)	EA+AE	[73086]
	11965.04	(0.05)	41(20,21)	-	41(20,22)	AA	[73086]
	11967.38	(0.05)	41(20,21)	-	41(20,22)	EE	[73086]
	11969.55	(0.05)	41(20,21)	-	41(20,22)	EA	[73086]
	11969.90	(0.05)	41(20,21)	-	41(20,22)	AE	[73086]
	12163.66	(0.05)	23(11,12)	-	23(11,13)	AA	[73086]
	12164.66	(0.05)	23(11,12)	-	23(11,13)	EE	[73086]
	12164.94	(0.05)	39(19,20)	-	39(19,21)	AA	[73086]
	12165.61	(0.05)	23(11,12)	-	23(11,13)	EA+AE	[73086]
	12167.18	(0.05)	39(19,20)	-	39(19,21)	EE	[73086]
	12169.23	(0.05)	39(19,20)	-	39(19,21)	EA	[73086]
	12169.53	(0.05)	39(19,20)	-	39(19,21)	AE	[73086]
	12330.47	(0.05)	37(18,19)	-	37(18,20)	AA	[73086]
	12332.54	(0.05)	37(18,19)	-	37(18,20)	EE	[73086]
	12334.46	(0.05)	37(18,19)	-	37(18,20)	EA	[73086]
	12334.81	(0.05)	37(18,19)	-	37(18,20)	AE	[73086]
	12338.75	(0.05)	6(2, 4)	-	6(4, 3)	EA+AE	[73086]
	12339.30	(0.05)	6(2, 4)	-	6(4, 3)	EE	[73086]
	12339.89	(0.05)	6(2, 4)	-	6(4, 3)	AA	[73086]
	12361.57	(0.05)	25(12,13)	-	25(12,14)	AA	[73086]
	12362.70	(0.05)	25(12,13)	-	25(12,14)	EE	[73086]
	12363.82	(0.05)	25(12,13)	-	25(12,14)	EA	[73086]
	12363.91	(0.05)	25(12,13)	-	25(12,14)	AE	[73086]
	12457.48	(0.05)	35(17,18)	-	35(17,19)	AA	[73086]
	12459.42	(0.05)	35(17,18)	-	35(17,19)	EE	[73086]
	12461.24	(0.05)	35(17,18)	-	35(17,19)	EA	[73086]
	12461.49	(0.05)	35(17,18)	-	35(17,19)	AE	[73086]
	12493.43	(0.05)	27(13,14)	-	27(13,15)	AA	[73086]
	12494.73	(0.05)	27(13,14)	-	27(13,15)	EE	[73086]
	12495.97	(0.05)	27(13,14)	-	27(13,15)	EA	[73086]
	12496.12	(0.05)	27(13,14)	-	27(13,15)	AE	[73086]
	12541.69	(0.05)	33(16,17)	-	33(16,18)	AA	[73086]
	12543.50	(0.05)	33(16,17)	-	33(16,18)	EE	[73086]
	12545.12	(0.05)	33(16,17)	-	33(16,18)	EA	[73086]
	12545.43	(0.05)	33(16,17)	-	33(16,18)	AE	[73086]
	12564.26	(0.05)	29(14,15)	-	29(14,16)	AA	[73086]
	12565.72	(0.05)	29(14,15)	-	29(14,16)	EE	[73086]
	12567.13	(0.05)	29(14,15)	-	29(14,16)	EA	[73086]
	12567.27	(0.05)	29(14,16)	-	29(14,15)	AE	[73086]
	12578.79	(0.05)	31(15,16)	-	31(15,17)	AA	[73086]
	12580.42	(0.05)	31(15,16)	-	31(15,17)	EE	[73086]
	12581.98	(0.05)	31(15,16)	-	31(15,17)	EA	[73086]
	12582.16	(0.05)	31(15,16)	-	31(15,17)	AE	[73086]

TABLE 83.2. Microwave spectrum of ortho-xylene — Continued

C₈H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Sym.	Ref.
	13515.960	(0.030)	4(2, 3) - 3(2, 2)		[73086]
	14249.350	(0.030)	5(1, 5) - 4(1, 4)		[73086]
	14292.463	(0.030)	5(0, 5) - 4(0, 4)		[73086]
	14471.229	(0.030)	4(1, 3) - 3(1, 2)		[73086]
	15125.10	(0.05)	9(3, 6) - 9(5, 5)	EA + AE	[73086]
	15125.75	(0.05)	9(3, 6) - 9(5, 5)	EE	[73086]
	15126.41	(0.05)	9(3, 6) - 9(5, 5)	AA	[73086]
	15339.59	(0.05)	16(7, 9) - 16(7, 10)	AA	[73086]
	15339.91	(0.05)	16(7, 9) - 16(7, 10)	EE	[73086]
	15340.10	(0.05)	16(7, 9) - 16(7, 10)	EA + AE	[73086]
	15363.90	(0.05)	8(3, 5) - 8(5, 4)	AE	[73086]
	15364.28	(0.05)	8(3, 5) - 8(5, 4)	EA	[73086]
	15364.91	(0.05)	8(3, 5) - 8(5, 4)	EE	[73086]
	15365.78	(0.05)	8(3, 5) - 8(5, 4)	AA	[73086]
	15556.680	(0.030)	4(2, 2) - 3(2, 1)		[73086]
	16479.525	(0.030)	5(2, 4) - 4(2, 3)		[73086]
	16861.91	(0.05)	20(9, 11) - 20(9, 12)	AA	[73086]
	16862.45	(0.05)	20(9, 11) - 20(9, 12)	EE	[73086]
	16863.04	(0.05)	20(9, 11) - 20(9, 12)	EA + AE	[73086]
	17476.54	(0.05)	22(10, 12) - 22(10, 13)	AA	[73086]
	17477.27	(0.05)	22(10, 12) - 22(10, 13)	EE	[73086]
	17477.99	(0.05)	22(10, 12) - 22(10, 13)	EA + AE	[73086]
	17999.82	(0.05)	24(11, 13) - 24(11, 14)	AA	[73086]
	18000.71	(0.05)	24(11, 13) - 24(11, 14)	EE	[73086]
	18001.63	(0.05)	24(11, 13) - 24(11, 14)	EA + AE	[73086]
	18435.88	(0.05)	26(12, 14) - 26(12, 15)	AA	[73086]
	18436.99	(0.05)	26(12, 14) - 26(12, 15)	EE	[73086]
	18438.08	(0.05)	26(12, 14) - 26(12, 15)	EA + AE	[73086]
	18578.68	(0.05)	48(23, 25) - 48(23, 26)	AA	[73086]
	18581.88	(0.05)	48(23, 25) - 48(23, 26)	EE	[73086]
	18585.01	(0.05)	48(23, 25) - 48(23, 26)	EA	[73086]
	18585.18	(0.05)	48(23, 25) - 48(23, 26)	AE	[73086]
	18788.80	(0.05)	28(13, 15) - 28(13, 16)	AA	[73086]
	18790.12	(0.05)	28(13, 15) - 28(13, 16)	EE	[73086]
	18791.40	(0.05)	28(13, 15) - 28(13, 16)	EA + AE	[73086]
	18848.52	(0.05)	46(22, 24) - 46(22, 25)	AA	[73086]
	18851.58	(0.05)	46(22, 24) - 46(22, 25)	EE	[73086]
	18854.56	(0.05)	46(22, 24) - 46(22, 25)	EA	[73086]
	18854.72	(0.05)	46(22, 24) - 46(22, 25)	AE	[73086]
	19062.45	(0.05)	30(14, 16) - 30(14, 17)	AA	[73086]
	19063.92	(0.05)	30(14, 16) - 30(14, 17)	EE	[73086]
	19065.43	(0.05)	30(14, 16) - 30(14, 17)	EA + AE	[73086]
	19073.36	(0.05)	44(21, 23) - 44(21, 24)	AA	[73086]
	19076.26	(0.05)	44(21, 23) - 44(21, 24)	EE	[73086]
	19079.17	(0.05)	44(21, 23) - 44(21, 24)	EA + AE	[73086]
	19249.32	(0.05)	42(20, 22) - 42(20, 23)	AA	[73086]
	19252.06	(0.05)	42(20, 22) - 42(20, 23)	EE	[73086]
	19254.73	(0.05)	42(20, 22) - 42(20, 23)	EA + AE	[73086]
	19260.52	(0.05)	32(15, 17) - 32(15, 18)	AA	[73086]
	19262.23	(0.05)	32(15, 17) - 32(15, 18)	EE	[73086]
	19263.96	(0.05)	32(15, 17) - 32(15, 18)	EA + AE	[73086]
	19372.52	(0.05)	40(19, 21) - 40(19, 22)	AA	[73086]
	19375.06	(0.05)	40(19, 21) - 40(19, 22)	EE	[73086]
	19377.56	(0.05)	40(19, 21) - 40(19, 22)	EA + AE	[73086]
	19386.78	(0.05)	34(16, 18) - 34(16, 19)	AA	[73086]
	19388.70	(0.05)	34(16, 18) - 34(16, 19)	EE	[73086]
	19390.68	(0.05)	34(16, 18) - 34(16, 19)	EA + AE	[73086]
	19439.05	(0.05)	38(18, 22) - 38(18, 21)	AA	[73086]
	19441.36	(0.05)	38(18, 22) - 38(18, 21)	EE	[73086]
	19443.68	(0.05)	38(18, 21) - 38(18, 20)	EA + AE	[73086]
	19445.11	(0.05)	36(17, 19) - 36(17, 20)	AA	[73086]
	19447.20	(0.05)	36(17, 19) - 36(17, 20)	EE	[73086]
	19449.31	(0.05)	36(17, 19) - 36(17, 20)	EA + AE	[73086]
	8995.630	(0.030)	3(0, 3) - 2(0, 2)		[73086]
	11144.060	(0.030)	3(1, 2) - 2(1, 1)		[73086]
	11349.395	(0.030)	4(1, 4) - 3(1, 3)		[73086]
	11372.54	(0.05)	28(14, 14) - 28(14, 15)	A	[73086]

C(CH₂D)(CH)₂CCH₃

TABLE 83.2. Microwave spectrum of ortho-xylene — Continued

C₈H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$	$- J''(K_{-1}, K_{+1})$	Sym.	Ref.
	11373.34	(0.05)	28(14,14)	- 28(14,15)	<i>E</i>	[73086]
	11460.800	(0.030)	4(0, 4)	- 3(0, 3)		[73086]
	11755.69	(0.05)	30(15,15)	- 30(15,16)	<i>A</i>	[73086]
	11756.64	(0.05)	30(15,15)	- 30(15,16)	<i>E</i>	[73086]
	12110.08	(0.05)	32(16,16)	- 32(16,17)	<i>A</i>	[73086]
	12111.20	(0.05)	32(16,16)	- 32(16,17)	<i>E</i>	[73086]
	12437.07	(0.05)	34(17,17)	- 34(17,18)	<i>A</i>	[73086]
	12438.25	(0.05)	34(17,17)	- 34(17,18)	<i>E</i>	[73086]
	12737.81	(0.05)	36(18,18)	- 36(18,19)	<i>A</i>	[73086]
	12739.12	(0.05)	36(18,18)	- 36(18,19)	<i>E</i>	[73086]
	13013.46	(0.05)	38(19,19)	- 38(19,20)	<i>A</i>	[73086]
	13014.87	(0.05)	38(19,19)	- 38(19,20)	<i>E</i>	[73086]
	13265.16	(0.05)	40(20,20)	- 40(20,21)	<i>A</i>	[73086]
	13266.62	(0.05)	40(20,20)	- 40(20,21)	<i>E</i>	[73086]
	13270.365	(0.030)	4(2, 3)	- 3(2, 2)		[73086]
	13493.79	(0.05)	42(21,21)	- 42(21,22)	<i>A</i>	[73086]
	13495.42	(0.05)	42(21,21)	- 42(21,22)	<i>E</i>	[73086]
	13700.40	(0.05)	44(22,22)	- 44(22,23)	<i>A</i>	[73086]
	13702.17	(0.05)	44(22,22)	- 44(22,23)	<i>E</i>	[73086]
	13885.95	(0.05)	46(23,23)	- 46(23,24)	<i>A</i>	[73086]
	13887.75	(0.05)	46(23,23)	- 46(23,24)	<i>E</i>	[73086]
	13928.385	(0.030)	5(1, 5)	- 4(1, 4)		[73086]
	13961.560	(0.030)	5(0, 5)	- 4(0, 4)		[73086]
	14051.19	(0.05)	48(24,24)	- 48(24,25)	<i>A</i>	[73086]
	14053.06	(0.05)	48(24,24)	- 48(24,25)	<i>E</i>	[73086]
	14165.080	(0.030)	4(1, 3)	- 3(1, 2)		[73086]
	15358.350	(0.030)	4(2, 2)	- 3(2, 1)		[73086]
	16148.740	(0.030)	5(2, 4)	- 4(2, 3)		[73086]
C(CDH ₂)(CH) ₄ CCH ₃	9036.500	(0.030)	3(0, 3)	- 2(0, 2)		[73086]
	9536.35	(0.05)	25(12,13)	- 25(12,14)	<i>+A</i>	[73086]
	9536.64	(0.05)	25(12,13)	- 25(12,14)	<i>-A</i>	[73086]
	9537.17	(0.05)	25(12,13)	- 25(12,14)	<i>+E</i>	[73086]
	9537.46	(0.05)	25(12,13)	- 25(12,14)	<i>-E</i>	[73086]
	11053.075	(0.030)	3(1, 2)	- 2(1, 1)		[73086]
	11371.620	(0.030)	4(1, 4)	- 3(1, 3)		[73086]
	11516.185	(0.030)	4(0, 4)	- 3(0, 3)		[73086]
	11757.51	(0.05)	46(22,24)	- 46(22,25)	<i>A</i>	[73086]
	11758.23	(0.05)	46(22,24)	- 46(22,25)	<i>E</i>	[73086]
	11759.47	(0.05)	46(22,24)	- 46(22,25)	<i>E</i>	[73086]
	11760.26	(0.05)	46(22,24)	- 46(22,25)	<i>E</i>	[73086]
	12795.34	(0.05)	42(20,22)	- 42(20,23)	<i>A</i>	[73086]
	12796.05	(0.05)	42(20,22)	- 42(20,23)	<i>A</i>	[73086]
	12797.21	(0.05)	42(20,22)	- 42(20,23)	<i>E</i>	[73086]
	12797.90	(0.05)	42(20,22)	- 42(20,23)	<i>E</i>	[73086]
	13200.820	(0.030)	4(2, 3)	- 3(2, 2)		[73086]
	13708.06	(0.05)	38(18,20)	- 38(18,21)	<i>A</i>	[73086]
	13708.70	(0.05)	38(18,20)	- 38(18,21)	<i>A</i>	[73086]
	13709.73	(0.05)	38(18,20)	- 38(18,21)	<i>E</i>	[73086]
	13710.37	(0.05)	38(18,20)	- 38(18,21)	<i>E</i>	[73086]
	13970.620	(0.030)	5(1, 5)	- 4(1, 4)		[73086]
	14019.235	(0.030)	5(0, 5)	- 4(0, 4)		[73086]
	14153.230	(0.030)	4(1, 3)	- 3(1, 2)		[73086]
	14913.30	(0.05)	30(14,16)	- 30(14,17)	<i>-A</i>	[73086]
	14913.76	(0.05)	30(14,16)	- 30(14,17)	<i>+A</i>	[73086]
	14914.45	(0.05)	30(14,16)	- 30(14,17)	<i>-E</i>	[73086]
	14914.98	(0.05)	30(14,16)	- 30(14,17)	<i>+E</i>	[73086]
	15080.73	(0.05)	26(12,14)	- 26(12,15)	<i>-A</i>	[73086]
	15081.10	(0.05)	26(12,14)	- 26(12,15)	<i>+A</i>	[73086]
	15081.62	(0.05)	26(12,14)	- 26(12,15)	<i>-E</i>	[73086]
	15081.92	(0.05)	26(12,14)	- 26(12,15)	<i>+E</i>	[73086]
	15128.935	(0.030)	4(2, 2)	- 3(2, 1)		[73086]
	16116.645	(0.030)	5(2, 4)	- 4(2, 3)		[73086]
C(CD ₂ H)(CH) ₄ CCH ₃	8868.410	(0.030)	3(0, 3)	- 2(0, 2)		[73086]
	9504.02	(0.05)	36(17,19)	- 36(17,20)	<i>A</i>	[73086]
	9505.02	(0.05)	36(17,19)	- 36(17,20)	<i>E</i>	[73086]
	10609.18	(0.05)	32(15,17)	- 32(15,18)	<i>A</i>	[73086]
	10610.04	(0.05)	32(15,17)	- 32(15,18)	<i>E</i>	[73086]

TABLE 83.2. Microwave spectrum of ortho-xylene — Continued

C₈H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Sym.	Ref.
	10784.050	(0.030)	3(1, 2) - 2(1, 1)		[73086]
	11099.82	(0.05)	30(14,16) - 30(14,17)	A	[73086]
	11100.58	(0.05)	30(14,16) - 30(14,17)	E	[73086]
	11151.940	(0.030)	4(1, 4) - 3(1, 3)		[73086]
	11307.060	(0.030)	4(0, 4) - 3(0, 3)		[73086]
	11531.90	(0.05)	28(13,15) - 28(13,16)	A	[73086]
	11532.59	(0.05)	28(13,15) - 28(13,16)	E	[73086]
	11753.66	(0.05)	47(22,25) - 47(22,26)	A	[73086]
	11755.16	(0.05)	47(22,25) - 47(22,26)	E	[73086]
	12561.81	(0.05)	45(21,24) - 45(21,25)	A	[73086]
	12563.24	(0.05)	45(21,24) - 45(21,25)	E	[73086]
	12900.850	(0.030)	4(2, 3) - 3(2, 2)		[73086]
	13355.68	(0.05)	43(20,23) - 43(20,24)	A	[73086]
	13357.07	(0.05)	43(20,23) - 43(20,24)	E	[73086]
	13707.940	(0.030)	5(1, 5) - 4(1, 4)		[73086]
	13762.460	(0.030)	5(0, 5) - 4(0, 4)		[73086]
	13847.890	(0.030)	4(1, 3) - 3(1, 2)		[73086]
	14123.10	(0.05)	41(19,22) - 41(19,23)	A	[73086]
	14124.46	(0.05)	41(19,22) - 41(19,23)	E	[73086]
	14719.355	(0.030)	4(2, 2) - 3(2, 1)		[73086]
	14851.23	(0.05)	39(18,21) - 39(18,22)	A	[73086]
	14852.49	(0.05)	39(18,21) - 39(18,22)	E	[73086]
	15527.05	(0.05)	37(17,20) - 37(17,21)	A	[73086]
	15528.23	(0.05)	37(17,20) - 37(17,21)	E	[73086]
	15771.220	(0.030)	5(2, 4) - 4(2, 3)		[73086]
C(CHD ₂)(CH) ₄ CCH ₃	8830.995	(0.030)	3(0, 3) - 2(0, 2)		[73086]
	10869.480	(0.030)	3(1, 2) - 2(1, 1)		[73086]
	11129.665	(0.030)	4(1, 4) - 3(1, 3)		[73086]
	11253.215	(0.030)	4(0, 4) - 3(0, 3)		[73086]
	12601.49	(0.05)	49(24,25) - 49(24,26)	A	[73086]
	12602.72	(0.05)	49(24,25) - 49(24,26)	E	[73086]
	12696.54	(0.05)	25(12,13) - 25(12,14)	A	[73086]
	12696.87	(0.05)	25(12,13) - 25(12,14)	E	[73086]
	12801.07	(0.05)	47(23,24) - 47(23,25)	A	[73086]
	12802.20	(0.05)	47(23,24) - 47(23,25)	E	[73086]
	12937.46	(0.05)	27(13,14) - 27(13,15)	A	[73086]
	12937.90	(0.05)	27(13,14) - 27(13,15)	E	[73086]
	12964.065	(0.030)	4(2, 3) - 3(2, 2)		[73086]
	12975.57	(0.05)	45(22,23) - 45(22,24)	A	[73086]
	12976.65	(0.05)	45(22,23) - 45(22,24)	E	[73086]
	13238.34	(0.05)	41(20,21) - 41(20,22)	A	[73086]
	13239.37	(0.05)	41(20,21) - 41(20,22)	E	[73086]
	13253.93	(0.05)	31(15,16) - 31(15,17)	A	[73086]
	13254.58	(0.05)	31(15,16) - 31(15,17)	E	[73086]
	13320.84	(0.05)	39(19,20) - 39(19,21)	A	[73086]
	13321.76	(0.05)	39(19,20) - 39(19,21)	E	[73086]
	13336.48	(0.05)	33(16,17) - 33(16,18)	A	[73086]
	13337.19	(0.05)	33(16,17) - 33(16,18)	E	[73086]
	13366.73	(0.05)	37(18,19) - 37(18,20)	A	[73086]
	13367.61	(0.05)	37(18,19) - 37(18,20)	E	[73086]
	13373.01	(0.05)	35(17,18) - 35(17,19)	A	[73086]
	13373.78	(0.05)	35(17,18) - 35(17,19)	E	[73086]
	13666.220	(0.030)	5(1, 5) - 4(1, 4)		[73086]
	13705.220	(0.030)	5(0, 5) - 4(0, 4)		[73086]
	13866.850	(0.030)	4(1, 3) - 3(1, 2)		[73086]
	14930.625	(0.030)	4(2, 2) - 3(2, 1)		[73086]
	15801.810	(0.030)	5(2, 4) - 4(2, 3)		[73086]
	19039.35	(0.05)	28(13,15) - 28(13,16)	A	[73086]
	19039.69	(0.05)	28(13,15) - 28(13,16)	E	[73086]
	19446.40	(0.05)	30(14,16) - 30(14,17)	A	[73086]
	19446.86	(0.05)	30(14,16) - 30(14,17)	E	[73086]
	19786.84	(0.05)	32(15,17) - 32(15,18)	A	[73086]
	19787.36	(0.05)	32(15,17) - 32(15,18)	E	[73086]
	20278.34	(0.05)	36(17,19) - 36(17,20)	A	[73086]
	20279.12	(0.05)	36(17,19) - 36(17,20)	E	[73086]
	20426.65	(0.05)	48(23,25) - 48(23,26)	A	[73086]
	20427.99	(0.05)	48(23,25) - 48(23,26)	E	[73086]

TABLE 83.2. Microwave spectrum of ortho-xylene — Continued

C₈H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Sym.	Ref.
	20434.72	(0.05)	38(18,20) - 38(18,21)	A	[73086]
	20435.59	(0.05)	38(18,20) - 38(18,21)	E	[73086]
	20524.83	(0.05)	46(22,24) - 46(22,25)	A	[73086]
	20526.04	(0.05)	46(22,24) - 46(22,25)	E	[73086]
	20534.96	(0.05)	40(19,21) - 40(19,22)	A	[73086]
	20535.86	(0.05)	40(19,21) - 40(19,22)	E	[73086]
	20577.32	(0.05)	44(21,23) - 44(21,24)	A	[73086]
	20578.43	(0.05)	44(21,23) - 44(21,24)	E	[73086]
	20581.61	(0.05)	42(20,22) - 42(20,23)	A	[73086]
	20582.58	(0.05)	42(20,22) - 42(20,23)	E	[73086]
	27978.61	(0.05)	39(18,21) - 39(18,22)	A	[73086]
	27979.20	(0.05)	39(18,21) - 39(18,22)	E	[73086]
	28331.98	(0.05)	41(19,22) - 41(19,23)	A	[73086]
	28332.68	(0.05)	41(19,22) - 41(19,23)	E	[73086]
	28845.58	(0.05)	45(21,24) - 45(21,25)	A	[73086]
	28846.49	(0.05)	45(21,24) - 45(21,25)	E	[73086]
	29009.12	(0.05)	47(22,25) - 47(22,26)	A	[73086]
	29010.15	(0.05)	47(22,25) - 47(22,26)	E	[73086]
	29112.71	(0.05)	49(23,26) - 49(23,27)	A	[73086]
	29113.84	(0.05)	49(23,26) - 49(23,27)	E	[73086]
C(CD ₃)(CH) ₄ CCH ₃	8674.545	(0.030)	3(0, 3) - 2(0, 2)		[73086]
	10607.030	(0.030)	3(1, 2) - 2(1, 1)		[73086]
	10921.870	(0.030)	4(1, 4) - 3(1, 3)		[73086]
	11057.650	(0.030)	4(0, 4) - 3(0, 3)		[73086]
	11674.71	(0.05)	48(23,25) - 48(23,26)	A	[73086]
	11675.39	(0.05)	48(23,25) - 48(23,26)	E	[73086]
	12171.00	(0.05)	46(22,24) - 46(22,25)	A	[73086]
	12171.66	(0.05)	46(22,24) - 46(22,25)	E	[73086]
	12645.24	(0.05)	44(21,23) - 44(21,24)	A	[73086]
	12645.86	(0.05)	44(21,23) - 44(21,24)	E	[73086]
	12673.115	(0.030)	4(2, 3) - 3(2, 2)		[73086]
	13091.28	(0.05)	42(20,22) - 42(20,23)	A	[73086]
	13091.85	(0.05)	42(20,22) - 42(20,23)	E	[73086]
	13418.680	(0.030)	5(1, 5) - 4(1, 4)		[73086]
	13463.935	(0.030)	4(2, 3) - 3(2, 2)		[73086]
	13502.63	(0.05)	40(19,21) - 40(19,22)	A	[73086]
	13503.13	(0.05)	40(19,21) - 40(19,22)	E	[73086]
	13578.925	(0.030)	4(1, 3) - 3(1, 2)		[73086]
	13872.70	(0.05)	38(18,20) - 38(18,21)	A	[73086]
	13873.15	(0.05)	38(18,20) - 38(18,21)	E	[73086]
C(¹³ CH ₃)(CH) ₄ CCH ₃	14194.74	(0.05)	36(17,19) - 36(17,20)	A	[73086]
	14195.10	(0.05)	36(17,19) - 36(17,20)	E	[73086]
	14522.960	(0.030)	4(2, 2) - 3(2, 1)		[73086]
	14667.82	(0.05)	32(15,17) - 32(15,18)	A	[73086]
	14668.03	(0.05)	32(15,17) - 32(15,18)	E	[73086]
	15471.275	(0.030)	5(2, 4) - 4(2, 3)		[73086]
	18848.91	(0.05)	49(23,26) - 49(23,27)	A	[73086]
	18849.55	(0.05)	49(23,26) - 49(23,27)	E	[73086]
	19371.95	(0.05)	47(22,25) - 47(22,26)	A	[73086]
	19372.62	(0.05)	47(22,25) - 47(22,26)	E	[73086]
	19842.05	(0.05)	45(21,24) - 45(21,25)	A	[73086]
	19842.61	(0.05)	45(21,24) - 45(21,25)	E	[73086]
	9087.510	(0.030)	3(0, 3) - 2(0, 2)		[73086]
	11175.090	(0.030)	3(1, 2) - 2(1, 1)		[73086]
	11443.445	(0.030)	4(1, 4) - 3(1, 3)		[73086]
	11577.075	(0.030)	4(0, 4) - 3(0, 3)		[73086]
	11784.97	(0.05)	37(18,19) - 37(18,20)	A	[73086]
	11786.53	(0.05)	37(18,19) - 37(18,20)	E ₁₀	[73086]
	11787.38	(0.05)	37(18,19) - 37(18,20)	E ₀₁	[73086]
	11788.81	(0.05)	37(18,19) - 37(18,20)	E ₁₋₁	[73086]
	11789.08	(0.05)	37(18,19) - 37(18,20)	E ₁₁	[73086]
	11935.55	(0.05)	35(17,18) - 35(17,19)	A	[73086]
	11937.02	(0.05)	35(17,18) - 35(17,19)	E ₁₀	[73086]
	11937.80	(0.05)	35(17,18) - 35(17,19)	E ₀₁	[73086]
	11939.15	(0.05)	35(17,18) - 35(17,19)	E ₁₋₁	[73086]
	11939.34	(0.05)	35(17,18) - 35(17,19)	E ₁₁	[73086]
	11975.40	(0.05)	25(12,13) - 25(12,14)	A	[73086]

TABLE 83.2. Microwave spectrum of ortho-xylene — Continued

C₈H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$	$- J''(K_{-1}, K_{+1})$	Sym.	Ref.
	11976.24	(0.05)	25(12,13)	- 25(12,14)	E_{10}	[73086]
	11976.72	(0.05)	25(12,13)	- 25(12,14)	E_{01}	[73086]
	11977.59	(0.05)	25(12,13)	- 25(12,14)	E_{1-1}	[73086]
	11977.59	(0.05)	25(12,13)	- 25(12,14)	E_{11}	[73086]
	12044.79	(0.05)	33(16,17)	- 33(16,18)	A	[73086]
	12046.16	(0.05)	33(16,17)	- 33(16,18)	E_{10}	[73086]
	12046.90	(0.05)	33(16,17)	- 33(16,18)	E_{01}	[73086]
	12048.14	(0.05)	33(16,17)	- 33(16,18)	E_{1-1}	[73086]
	12048.37	(0.05)	33(16,17)	- 33(16,18)	E_{11}	[73086]
	12078.37	(0.05)	27(13,14)	- 27(13,15)	A	[73086]
	12079.37	(0.05)	27(13,14)	- 27(13,15)	E_{10}	[73086]
	12079.92	(0.05)	27(13,14)	- 27(13,15)	E_{01}	[73086]
	12080.90	(0.05)	27(13,14)	- 27(13,15)	E_{1-1}	[73086]
	12080.90	(0.05)	27(13,14)	- 27(13,15)	E_{11}	[73086]
	12108.26	(0.05)	31(15,16)	- 31(15,17)	A	[73086]
	12109.47	(0.05)	31(15,16)	- 31(15,17)	E_{10}	[73086]
	12110.10	(0.05)	31(15,16)	- 31(15,17)	E_{01}	[73086]
	12111.32	(0.05)	31(15,16)	- 31(15,17)	E_{1-1}	[73086]
	12111.47	(0.05)	31(15,16)	- 31(15,17)	E_{11}	[73086]
	12120.98	(0.05)	29(14,15)	- 29(14,16)	A	[73086]
	12122.09	(0.05)	29(14,15)	- 29(14,16)	E_{10}	[73086]
	12122.70	(0.05)	29(14,15)	- 29(14,16)	E_{01}	[73086]
	12123.82	(0.05)	29(14,15)	- 29(14,16)	E_{1-1}	[73086]
	12123.82	(0.05)	29(14,15)	- 29(14,16)	E_{11}	[73086]
	13326.695	(0.030)	4(2, 3)	- 3(2, 2)		[73086]
	14052.205	(0.030)	5(1, 5)	- 4(1, 4)		[73086]
	14095.255	(0.030)	5(0, 5)	- 4(0, 4)		[73086]
	14271.110	(0.030)	4(1, 3)	- 3(1, 2)		[73086]
	15335.000	(0.030)	4(2, 2)	- 3(2, 1)		[73086]
	16250.270	(0.030)	5(2, 4)	- 4(2, 3)		[73086]
C(CH ₃)CD(CH ₃)CCH ₃	9049.980	(0.030)	3(0, 3)	- 2(0, 2)		[73086]
	11239.680	(0.030)	3(1, 2)	- 2(1, 1)		[73086]
	11425.810	(0.030)	4(1, 4)	- 3(1, 3)		[73086]
	11531.020	(0.030)	4(0, 4)	- 3(0, 3)		[73086]
	12627.19	(0.05)	26(13,13)	- 26(13,14)	A	[73086]
	12628.22	(0.05)	26(13,13)	- 26(13,14)	E_{10}	[73086]
	12628.57	(0.05)	26(13,13)	- 26(13,14)	E_{01}	[73086]
	12629.63	(0.05)	26(13,13)	- 26(13,14)	E_{1-1}	[73086]
	12629.63	(0.05)	26(13,13)	- 26(13,14)	E_{11}	[73086]
	13249.18	(0.05)	28(14,14)	- 28(14,15)	A	[73086]
	13250.29	(0.05)	28(14,14)	- 28(14,15)	E_{10}	[73086]
	13250.86	(0.05)	28(14,14)	- 28(14,15)	E_{01}	[73086]
	13252.02	(0.05)	28(14,14)	- 28(14,15)	E_{1-1}	[73086]
	13252.02	(0.05)	28(14,14)	- 28(14,15)	E_{11}	[73086]
	13378.005	(0.030)	4(2, 3)	- 3(2, 2)		[73086]
	14019.450	(0.030)	5(1, 5)	- 4(1, 4)		[73086]
	14049.870	(0.030)	5(0, 5)	- 4(0, 4)		[73086]
	14262.320	(0.030)	4(1, 3)	- 3(1, 2)		[73086]
	14429.51	(0.05)	32(16,16)	- 32(16,17)	A	[73086]
	14431.04	(0.05)	32(16,16)	- 32(16,17)	E_{10}	[73086]
	14431.56	(0.05)	32(16,16)	- 32(16,17)	E_{01}	[73086]
	14433.03	(0.05)	32(16,16)	- 32(16,17)	E_{1-1}	[73086]
	14433.03	(0.05)	32(16,16)	- 32(16,17)	E_{11}	[73086]
	14989.51	(0.05)	34(17,17)	- 34(17,18)	A	[73086]
	14991.13	(0.05)	34(17,17)	- 34(17,18)	E_{10}	[73086]
	14991.78	(0.05)	34(17,17)	- 34(17,18)	E_{01}	[73086]
	15513.190	(0.030)	4(2, 2)	- 3(2, 1)		[73086]
	15530.59	(0.05)	36(18,18)	- 36(18,19)	A	[73086]
	15532.58	(0.05)	36(18,18)	- 36(18,19)	E_{10}	[73086]
	15533.15	(0.05)	36(18,18)	- 36(18,19)	E_{01}	[73086]
	15534.82	(0.05)	36(18,18)	- 36(18,19)	E_{1-1}	[73086]
	15534.82	(0.05)	36(18,18)	- 36(18,19)	E_{11}	[73086]
	16268.005	(0.030)	5(2, 4)	- 4(2, 3)		[73086]
C(CH ₃)CHCDCHCHCCH ₃	9000.650	(0.030)	3(0, 3)	- 2(0, 2)		[73086]
	10997.105	(0.030)	3(1, 2)	- 2(1, 1)		[73086]
	11315.665	(0.030)	4(1, 4)	- 3(1, 3)		[73086]
	11467.660	(0.030)	4(0, 4)	- 3(0, 3)		[73086]

TABLE 83.2. Microwave spectrum of ortho-xylene — Continued

C₈H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Sym.	Ref.
	13132.360	(0.030)	4(2, 3) - 3(2, 2)		[73086]
	13902.900	(0.030)	5(1, 5) - 4(1, 4)		[73086]
	13995.140	(0.030)	5(0, 5) - 4(0, 4)		[73086]
	14096.880	(0.030)	4(1, 3) - 3(1, 2)		[73086]
	15034.550	(0.030)	4(2, 2) - 3(2, 1)		[73086]
	16040.135	(0.030)	5(2, 4) - 4(2, 3)		[73086]
	19652.46	(0.05)	25(11,14) - 25(11,15)	<i>A</i>	[73086]
	19652.94	(0.05)	25(11,14) - 25(11,15)	<i>E</i> ₁₀	[73086]
	19653.51	(0.05)	25(11,14) - 25(11,15)	<i>E</i> ₀₁	[73086]
	19654.07	(0.05)	25(11,14) - 25(11,15)	<i>E</i> ₁₋₁	[73086]
	19654.07	(0.05)	25(11,14) - 25(11,15)	<i>E</i> ₁₁	[73086]
	19751.77	(0.05)	29(13,16) - 29(13,17)	<i>A</i>	[73086]
	19752.58	(0.05)	29(13,16) - 29(13,17)	<i>E</i> ₁₀	[73086]
	19753.32	(0.05)	29(13,16) - 29(13,17)	<i>E</i> ₀₁	[73086]
	19754.23	(0.05)	29(13,16) - 29(13,17)	<i>E</i> ₁₋₁	[73086]
	19754.23	(0.05)	29(13,16) - 29(13,17)	<i>E</i> ₁₁	[73086]
	19763.89	(0.05)	27(12,15) - 27(12,16)	<i>A</i>	[73086]
	19764.59	(0.05)	27(12,15) - 27(12,16)	<i>E</i> ₁₀	[73086]
	19765.27	(0.05)	27(12,15) - 27(12,16)	<i>E</i> ₀₁	[73086]
	19765.91	(0.05)	27(12,15) - 27(12,16)	<i>E</i> ₁₋₁	[73086]
	19765.91	(0.05)	27(12,15) - 27(12,16)	<i>E</i> ₁₁	[73086]

Table 84.1. Molecular constants of bicyclo[2.2.2]octadiene.

Parameter	Value
<i>A</i> (MHz)	2730.114(2)
<i>B</i> (MHz)	2650.520(2)
<i>C</i> (MHz)	2631.712(2)
<i>D_J</i> (MHz)	0.000212(20)
<i>μ_C</i> (D)	0.432(2)

TABLE 84.2. Microwave spectrum of bicyclo(2.2.2)octadiene

C₈H₁₀


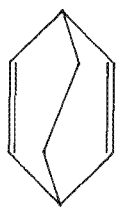
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
CHCHCHCHCHCH ₂ CH ₂	26656.46	(0.05)	5(1, 4) - 4(0, 4)	[83059]
	26669.20	(0.05)	5(2, 3) - 4(1, 3)	[83059]
	26770.07	(0.05)	5(2, 4) - 4(1, 4)	[83059]
	26840.26	(0.05)	5(3, 2) - 4(2, 2)	[83059]
	26872.65	(0.05)	5(3, 3) - 4(2, 3)	[83059]
	27034.25	(0.05)	5(4, 1) - 4(3, 1)	[83059]
	27036.07	(0.05)	5(4, 2) - 4(3, 2)	[83059]
	27212.55	(0.05)	5(5, 1) - 4(4, 1)	[83059]
	31085.02	(0.05)	6(3, 4) - 5(4, 2)	[83059]
	31203.62	(0.05)	6(1, 6) - 5(2, 4)	[83059]
	31211.95	(0.05)	6(2, 5) - 5(3, 3)	[83059]
	31337.09	(0.05)	6(0, 6) - 5(1, 4)	[83059]
	31354.03	(0.05)	6(2, 4) - 5(3, 2)	[83059]
	31490.92	(0.05)	6(1, 5) - 5(2, 3)	[83059]
	31972.19	(0.05)	6(2, 4) - 5(1, 4)	[83059]
	32008.61	(0.05)	6(1, 5) - 5(0, 5)	[83059]
	32096.42	(0.05)	6(2, 5) - 5(1, 5)	[83059]
	32108.11	(0.05)	6(3, 3) - 5(2, 3)	[83059]
	32170.72	(0.05)	6(3, 4) - 5(2, 4)	[83059]
	32313.75	(0.05)	6(4, 2) - 5(3, 2)	[83059]
	32320.56	(0.05)	6(4, 3) - 5(3, 3)	[83059]
	32495.52	(0.05)	6(5, 2) - 5(4, 2)	[83059]
	32672.71	(0.05)	6(6, 1) - 5(5, 1)	[83059]
	36367.61	(0.05)	7(3, 5) - 6(4, 3)	[83059]
	36408.46	(0.05)	7(1, 7) - 6(2, 5)	[83059]
	36418.16	(0.05)	7(3, 4) - 6(4, 2)	[83059]
	36462.63	(0.05)	7(2, 6) - 6(3, 4)	[83059]
	36508.14	(0.05)	7(0, 7) - 6(1, 5)	[83059]
	36673.52	(0.05)	7(2, 5) - 6(3, 3)	[83059]
	36733.34	(0.05)	7(1, 6) - 6(2, 4)	[83059]
	37290.68	(0.05)	7(2, 5) - 6(1, 5)	[83059]
	37368.42	(0.05)	7(1, 6) - 6(0, 6)	[83059]
	37377.83	(0.05)	7(3, 4) - 6(2, 4)	[83059]
	37429.73	(0.05)	7(2, 6) - 6(1, 6)	[83059]
	37476.18	(0.05)	7(3, 5) - 6(2, 5)	[83059]
	37588.27	(0.05)	7(4, 3) - 6(3, 3)	[83059]
	37606.95	(0.05)	7(4, 4) - 6(3, 4)	[83059]
	37777.58	(0.05)	7(5, 2) - 6(4, 2)	[83059]
	37778.48	(0.05)	7(5, 3) - 6(4, 3)	[83059]
	37955.71	(0.05)	7(6, 2) - 6(5, 2)	[83059]
	38132.85	(0.05)	7(7, 1) - 6(6, 1)	[83059]

Table 85.1. Molecular constants of bicyclo[2.2.2]octene.

Parameter	Value
A (MHz)	2576.737(4)
B (MHz)	2509.013(4)
C (MHz)	2462.283(8)
D _J (MHz)	0.000178(46)
μ _C (D)	0.253(1)

TABLE 85.2. Microwave spectrum of bicyclo(2.2.2.)octene

C₈H₁₂

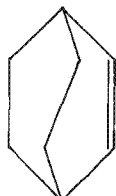
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
$\text{CHCH}_2\text{CH}_2\text{CHCH}_2\text{CH}_2\text{CHCH}$ 	30293.93	(0.05)	6(3, 3) - 5(2, 3)	[83059]
	30313.10	(0.05)	6(2, 4) - 5(1, 4)	[83059]
	30393.53	(0.05)	6(1, 5) - 5(0, 5)	[83059]
	30408.65	(0.05)	6(2, 5) - 5(1, 5)	[83059]
	30419.60	(0.05)	6(3, 4) - 5(2, 4)	[83059]
	30446.99	(0.05)	6(4, 2) - 5(3, 2)	[83059]
	30504.88	(0.05)	6(4, 3) - 5(3, 3)	[83059]
	30652.44	(0.05)	6(5, 1) - 5(4, 1)	[83059]
	30658.14	(0.05)	6(5, 2) - 5(4, 2)	[83059]
	30832.57	(0.05)	6(6, 0) - 5(5, 0)	[83059]
	30832.57	(0.05)	6(6, 1) - 5(5, 1)	[83059]
	35326.13	(0.05)	7(3, 4) - 6(2, 4)	[83059]
	35405.13	(0.05)	7(4, 3) - 6(3, 3)	[83059]
	35406.06	(0.05)	7(2, 5) - 6(1, 5)	[83059]
	35467.07	(0.05)	7(3, 5) - 6(2, 5)	[83059]
	35616.83	(0.05)	7(5, 2) - 6(4, 2)	[83059]
	35640.53	(0.05)	7(5, 3) - 6(4, 3)	[83059]
	35808.52	(0.05)	7(6, 1) - 6(5, 1)	[83059]
	35809.88	(0.05)	7(6, 2) - 6(5, 2)	[83059]
	35985.97	(0.05)	7(7, 1) - 6(6, 1)	[83059]
35985.97	(0.05)	7(7, 0) - 6(6, 0)	[83059]	

Table 86.1. Molecular constants of axial and equatorial ethynyl cyclohexane in the ground and lowest vibrational states.

Parameter	Equatorial		Axial
	Ground State [present]	$\nu_{54} = 1^a$	Ground State [present]
A (MHz)	4246.15(10)	4194.6(1)	2994.441(6)
B (MHz)	1386.4511(16)	1387.459(2)	1730.834(8)
C (MHz)	1121.7067(13)	1122.864(2)	1540.004(5)
E (cm ⁻¹) ^a	0	130.(30)	600.(200)

^aFrom reference [80036].

TABLE 86.2. Microwave spectrum of ethynyl cyclohexane

C₆H₁₂

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$	-	$J''(K_{-1}, K_{+1})$	Vib. state	Ref.
<i>eq</i> -CH(CCH)(CH ₂) ₄ CH ₂	18736.47	(0.05)	8(1, 8)	-	7(1, 7)		[80036]
	18982.46	(0.05)	8(0, 8)	-	7(0, 7)		[80036]
	19853.92	(0.05)	8(2, 7)	-	7(2, 6)		[80036]
	20682.82	(0.05)	8(1, 7)	-	7(1, 6)		[80036]
	20928.65	(0.05)	8(2, 6)	-	7(2, 5)		[80036]
	21018.17	(0.05)	9(1, 9)	-	8(1, 8)		[80036]
	21199.38	(0.05)	9(0, 9)	-	8(0, 8)		[80036]
	22265.20	(0.05)	9(2, 8)	-	8(2, 7)		[80036]
	23100.03	(0.05)	9(1, 8)	-	8(1, 7)		[80036]
	23289.35	(0.05)	10(1,10)	-	9(1, 9)		[80036]
	23416.70	(0.05)	10(0,10)	-	9(0, 9)		[80036]
	23620.02	(0.05)	9(2, 7)	-	8(2, 6)		[80036]
	24654.40	(0.05)	10(2, 9)	-	9(2, 8)		[80036]
	25452.95	(0.05)	10(1, 9)	-	9(1, 8)		[80036]
	25552.28	(0.05)	11(1,11)	-	10(1,10)		[80036]
	25638.61	(0.05)	11(0,11)	-	10(0,10)		[80036]
	26278.30	(0.05)	10(2, 8)	-	9(2, 7)		[80036]
	18990.20	(0.05)	8(0, 8)	-	7(0, 7)	1ν ₅₄	[80036]
	20951.73	(0.05)	8(2, 6)	-	7(2, 5)	1ν ₅₄	[80036]
	20212.83	(0.05)	8(3, 6)	-	7(3, 5)	1ν ₅₄	[80036]
	20389.58	(0.05)	8(3, 5)	-	7(3, 4)	1ν ₅₄	[80036]
	23105.67	(0.05)	9(1, 8)	-	8(1, 7)	1ν ₅₄	[80036]
	22279.78	(0.05)	9(2, 8)	-	8(2, 7)	1ν ₅₄	[80036]
	23643.27	(0.05)	9(2, 7)	-	8(2, 6)	1ν ₅₄	[80036]
	23052.40	(0.05)	9(3, 6)	-	8(3, 5)	1ν ₅₄	[80036]
	23429.22	(0.05)	10(0,10)	-	9(0, 9)	1ν ₅₄	[80036]
	23306.97	(0.05)	10(1,10)	-	9(1, 9)	1ν ₅₄	[80036]
	25455.76	(0.05)	10(1, 9)	-	9(1, 8)	1ν ₅₄	[80036]
	24669.48	(0.05)	10(2, 9)	-	9(2, 8)	1ν ₅₄	[80036]
	26300.45	(0.05)	10(2, 8)	-	9(2, 7)	1ν ₅₄	[80036]
	25653.93	(0.05)	11(0,11)	-	10(0,10)	1ν ₅₄	[80036]
	<i>ax</i> -CH(CCH)(CH ₂) ₄ CH ₂	16006.79	(0.10)	5(0, 5)	-	4(0, 4)	
16309.80		(0.10)	5(2, 4)	-	4(2, 3)		[80036]
16656.63		(0.10)	5(2, 3)	-	4(2, 2)		[80036]
16729.22		(0.10)	5(1, 4)	-	4(1, 3)		[80036]
18925.33		(0.10)	6(1, 6)	-	5(1, 5)		[80036]
19535.65		(0.10)	6(2, 5)	-	5(2, 4)		[80036]
19999.90		(0.10)	6(1, 5)	-	5(1, 4)		[80036]
22035.94		(0.10)	7(1, 7)	-	6(1, 6)		[80036]
22146.35		(0.10)	7(0, 7)	-	6(0, 6)		[80036]
22743.08		(0.10)	7(2, 6)	-	6(2, 5)		[80036]
22991.16		(0.10)	7(3, 5)	-	6(3, 4)		[80036]
22992.29		(0.10)	7(4, 4)	-	6(4, 3)		[80036]
23221.32		(0.10)	7(1, 6)	-	6(1, 5)		[80036]
25136.42		(0.10)	8(1, 8)	-	7(1, 7)		[80036]
25207.28		(0.10)	8(0, 8)	-	7(0, 7)		[80036]
25624.05		(0.10)	16(10, 7)	-	16(9, 7)		[80036]
25657.05		(0.10)	15(10, 6)	-	15(9, 6)		[80036]
26384.90		(0.10)	8(1, 7)	-	7(1, 6)		[80036]

Table 87.1. Molecular constants of indene.

Parameter	Value
A (MHz)	3775.012(49)
B (MHz)	1580.859(2)
C (MHz)	1122.241(2)

TABLE 87.2. Microwave spectrum of indene

C₉H₈


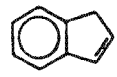
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
CH ₂ CHCHC(CH ₃) ₂ C 	21289.48	(0.10)	9(1, 9) - 8(1, 8)	[79036]
	21329.78	(0.10)	9(0, 9) - 8(0, 8)	[79036]
	23542.28	(0.10)	10(1,10) - 9(1, 9)	[79036]
	23562.72	(0.10)	10(0,10) - 9(0, 9)	[79036]
	23848.22	(0.10)	9(1, 8) - 8(1, 7)	[79036]
	24512.85	(0.10)	9(3, 7) - 8(3, 6)	[79036]
	24833.02	(0.10)	9(4, 6) - 8(4, 5)	[79036]
	25120.88	(0.10)	9(4, 5) - 8(4, 4)	[79036]
	25620.63	(0.10)	10(2, 9) - 9(2, 8)	[79036]
	25984.01	(0.10)	9(2, 7) - 8(2, 6)	[79036]
	26002.40	(0.10)	10(1, 9) - 9(1, 8)	[79036]
	26062.50	(0.10)	9(3, 6) - 8(3, 5)	[79036]

Table 88.1. Rotational analysis of azulene in the ground vibrational state.

Parameter	Value [present]
A'' (MHz)	2841.9543(59)
B'' (MHz)	1254.8449(32)
C'' (MHz)	870.7147(29)
τ_1 (kHz)	-1.018(800)
τ_2 (kHz)	-0.272(250)
τ_3^a (kHz)	3.33(200)
τ_{aaaa} (kHz)	0.17(130)
τ_{bbbb} (kHz)	-0.025(22)
τ_{cccc} (kHz)	-0.068(214)

^aValue fixed by setting $R_6 = 0$.

Table 88.2. Molecular constants for azulene in the ground and excited vibrational states. [72069]

Parameter	Ground	Vibrational State		
		$\nu_{2,3} = 1$	$\nu_{2,3} = 2$	$\nu_{4,8} = 1$
A (MHz)	2841.9531(29)	2841.7902(79)	2841.6294(150)	2836.6936(94)
B (MHz)	1254.8449(13)	1254.7722(19)	1254.7076(27)	1255.6163(21)
C (MHz)	870.7148(10)	871.4697(15)	872.2276(21)	871.4793(16)
τ_{aaaa} (kHz)	-0.417(367)	-1.839(612)	0.084(988)	-3.747(815)
τ_{bbbb} (kHz)	-0.281(79)	-0.161(126)	-0.411(184)	0.272(140)
τ_{aabb} (kHz)	-0.553(440)	0.073(734)	-1.280(1078)	2.543(815)
τ_{abab} (kHz)	0.029(175)	-0.019(342)	0.248(560)	-0.979(406)
E (cm ⁻¹)	0	188.0(24)	---	180.3(19)

Parameter	Ground	Vibrational State		
		$\nu_{4,8} = 2$	$\nu_{2,3} = 1,$ $\nu_{4,8} = 1$	$\nu_{4,7} = 1$
A (MHz)		2831.5965(105)	2836.5937(157)	2838.6659(107)
B (MHz)		1256.4039(19)	1255.5593(31)	1254.9585(25)
C (MHz)		872.2323(16)	872.2439(23)	871.2620(18)
τ_{aaaa} (kHz)		-2.296(645)	2.341(978)	-0.836(154)
τ_{bbbb} (kHz)		0.011(129)	-0.605(200)	0.229(154)
τ_{aabb} (kHz)		1.539(755)	-2.730(1151)	2.283(884)
τ_{abab} (kHz)		-1.249(405)	1.031(590)	-1.515(379)
E (cm ⁻¹)		---	---	272.7(50)

Electric Dipole Moment [65034]

μ_a (gnd)	0.796(14) D
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TABLE 88.3. Microwave spectrum of azulene

C₁₀H₈

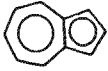
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1})$	$- J''(K_{-1}, K_{+1})$	Vib. state	Ref.
CHCHCHC(CH) ₂ C	7427.72	(0.02)	45(14,31)	- 45(14,32)		[72069]
	7439.68	(0.02)	68(21,47)	- 68(21,48)		[72069]
	7466.79	(0.03)	29(9,20)	- 29(9,21)	2ν ₂₃	[72069]
	7544.63	(0.02)	29(9,20)	- 29(9,21)	1ν ₂₃	[72069]
	7587.14	(0.02)	78(24,54)	- 78(24,55)		[72069]
	7623.17	(0.02)	29(9,20)	- 29(9,21)		[72069]
	7627.23	(0.02)	4(1, 4)	- 3(1, 3)		[72069]
	7630.83	(0.03)	4(1, 4)	- 3(1, 3)	1ν ₄₇	[72069]
	7632.03	(0.02)	4(1, 4)	- 3(1, 3)	1ν ₂₃	[72069]
	7633.08	(0.02)	4(1, 4)	- 3(1, 3)	1ν ₄₈	[72069]
	7636.80	(0.03)	4(1, 4)	- 3(1, 3)	2ν ₂₃	[72069]
	7637.90	(0.03)	4(1, 4)	- 3(1, 3)	1ν ₂₃	1ν ₄₈ [72069]
	7638.84	(0.03)	4(1, 4)	- 3(1, 3)	2ν ₄₈	[72069]
	7644.60	(0.03)	29(9,20)	- 29(9,21)	1ν ₄₇	[72069]
	7648.00	(0.02)	11(3, 8)	- 11(3, 9)	1ν ₂₃	1ν ₄₈ [72069]
	7657.98	(0.03)	29(9,20)	- 29(9,21)	1ν ₂₃	[72069]
	7674.82	(0.02)	11(3, 8)	- 11(3, 9)		[72069]
	7693.83	(0.02)	11(3, 8)	- 11(3, 9)	1ν ₄₈	[72069]
	7737.82	(0.02)	29(9,20)	- 29(9,21)	1ν ₄₈	[72069]
	7854.00	(0.03)	29(9,20)	- 29(9,21)	2ν ₄₈	[72069]
	7895.34	(0.03)	26(8,18)	- 26(8,19)	2ν ₂₃	[72069]
	7962.30	(0.02)	4(0, 4)	- 3(0, 3)		[72069]
	7965.22	(0.03)	4(0, 4)	- 3(0, 3)	1ν ₄₇	[72069]
	7966.42	(0.02)	26(8,18)	- 26(8,19)	1ν ₂₃	[72069]
	7966.97	(0.02)	4(0, 4)	- 3(0, 3)	1ν ₂₃	[72069]
	7967.05	(0.02)	4(0, 4)	- 3(0, 3)	1ν ₄₈	[72069]
	8028.64	(0.02)	55(17,38)	- 55(17,39)		[72069]
	8038.11	(0.02)	26(8,18)	- 26(8,19)		[72069]
	8055.28	(0.03)	26(8,18)	- 26(8,19)	1ν ₄₇	[72069]
	8062.31	(0.02)	42(13,29)	- 42(13,30)	1ν ₂₃	[72069]
	8138.23	(0.02)	26(8,18)	- 26(8,19)	1ν ₄₈	[72069]
	8163.23	(0.02)	14(4,10)	- 14(4,11)	1ν ₂₃	[72069]
	8184.81	(0.02)	42(13,29)	- 42(13,30)		[72069]
	8196.55	(0.03)	14(4,10)	- 14(4,11)	1ν ₂₃	1ν ₄₈ [72069]
	8199.06	(0.02)	14(4,10)	- 14(4,11)		[72069]
	8211.88	(0.03)	23(7,16)	- 23(7,17)	2ν ₂₃	[72069]
	8232.45	(0.02)	14(4,10)	- 14(4,11)	1ν ₄₈	[72069]
	8239.34	(0.03)	26(8,18)	- 26(8,19)	2ν ₄₈	[72069]
	8253.42	(0.03)	42(13,29)	- 42(13,30)	1ν ₂₃	1ν ₄₈ [72069]
	8266.14	(0.03)	14(4,10)	- 14(4,11)	2ν ₄₈	[72069]
	8274.99	(0.02)	23(7,16)	- 23(7,17)	1ν ₂₃	[72069]
	8338.55	(0.02)	23(7,16)	- 23(7,17)		[72069]
	8351.14	(0.03)	23(7,16)	- 23(7,17)	1ν ₄₇	[72069]
	8358.24	(0.03)	23(7,16)	- 23(7,17)	1ν ₂₃	1ν ₄₈ [72069]
	8366.34	(0.03)	17(5,12)	- 17(5,13)	2ν ₂₃	[72069]
	8381.25	(0.03)	20(6,14)	- 20(6,15)	2ν ₂₃	[72069]
	8411.30	(0.02)	17(5,12)	- 17(5,13)	1ν ₂₃	[72069]
	8421.21	(0.02)	65(20,45)	- 65(20,46)		[72069]
	8422.44	(0.02)	23(7,16)	- 23(7,17)	1ν ₄₈	[72069]
	8435.53	(0.02)	20(6,14)	- 18(6,15)	1ν ₂₃	[72069]
	8453.94	(0.02)	4(2, 3)	- 3(2, 2)		[72069]
	8456.53	(0.02)	17(5,12)	- 17(5,13)		[72069]
	8456.87	(0.02)	4(2, 3)	- 3(2, 2)	1ν ₂₃	[72069]
	8458.84	(0.03)	4(2, 3)	- 3(2, 2)	2ν ₂₃	[72069]
	8459.96	(0.02)	4(2, 3)	- 3(2, 2)	1ν ₄₈	[72069]
	8460.65	(0.03)	17(5,12)	- 17(5,13)	1ν ₂₃	1ν ₄₈ [72069]
	8465.94	(0.03)	4(2, 3)	- 3(2, 2)	2ν ₄₈	[72069]
	8490.13	(0.02)	20(6,14)	- 20(6,15)		[72069]
	8498.04	(0.03)	20(6,14)	- 20(6,15)	1ν ₄₇	[72069]
	8501.87	(0.03)	20(6,14)	- 20(6,15)	1ν ₂₃	1ν ₄₈ [72069]
	8506.11	(0.02)	17(5,12)	- 17(5,13)	1ν ₄₈	[72069]
	8506.96	(0.03)	23(7,16)	- 23(7,17)	2ν ₄₈	[72069]
	8556.06	(0.03)	17(5,12)	- 17(5,13)	2ν ₄₈	[72069]
	8556.86	(0.02)	20(6,14)	- 20(6,15)	1ν ₄₈	[72069]
	8608.96	(0.02)	4(3, 2)	- 3(3, 1)		[72069]
	8611.30	(0.02)	4(3, 2)	- 3(3, 1)	1ν ₂₃	[72069]
	8613.65	(0.03)	4(3, 2)	- 3(3, 1)	2ν ₂₃	[72069]

TABLE 88.3. Microwave spectrum of azulene — Continued

C₁₀H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	8615.45	(0.02)	4(3, 2) - 3(3, 1)	1ν ₄₈	[72069]
	8624.04	(0.03)	20(6, 14) - 20(6, 15)	2ν ₄₈	[72069]
	8640.30	(0.02)	75(23,52) - 75(23,53)		[72069]
	8645.97	(0.02)	4(3, 1) - 3(3, 0)		[72069]
	8648.12	(0.02)	4(3, 1) - 3(3, 0)	1ν ₂₃	[72069]
	8648.63	(0.03)	4(3, 1) - 3(3, 0)	1ν ₄₇	[72069]
	8650.26	(0.03)	4(3, 1) - 3(3, 0)	2ν ₂₃	[72069]
	8652.75	(0.02)	4(3, 1) - 3(3, 0)	1ν ₄₈	[72069]
	8808.69	(0.02)	39(12,27) - 39(12,28)	1ν ₂₃	[72069]
	8928.08	(0.02)	39(12,28) - 39(12,27)		[72069]
	8948.02	(0.02)	52(16,36) - 52(16,37)		[72069]
	8966.70	(0.03)	39(12,27) - 39(12,28)	1ν ₄₇	[72069]
	8993.34	(0.02)	4(2, 2) - 3(2, 1)		[72069]
	8994.34	(0.02)	4(2, 2) - 3(2, 1)	1ν ₂₃	[72069]
	8995.37	(0.03)	4(2, 2) - 3(2, 1)	2ν ₂₃	[72069]
	8995.79	(0.03)	4(2, 2) - 3(2, 1)	1ν ₄₇	[72069]
	9000.76	(0.02)	4(2, 2) - 3(2, 1)	1ν ₄₈	[72069]
	9001.82	(0.03)	4(2, 2) - 3(2, 1)	1ν ₂₃ 1ν ₄₈	[72069]
	9008.17	(0.03)	4(2, 2) - 3(2, 1)	2ν ₄₈	[72069]
	9041.16	(0.02)	9(2, 7) - 9(2, 8)	1ν ₂₃	[72069]
	9063.81	(0.02)	9(2, 8) - 9(2, 7)		[72069]
	9069.71	(0.02)	9(2, 7) - 9(2, 8)	1ν ₄₈	[72069]
	9113.46	(0.02)	39(12,27) - 39(12,28)	1ν ₄₈	[72069]
	9126.72	(0.02)	4(1, 3) - 3(1, 2)		[72069]
	9128.43	(0.02)	4(1, 3) - 3(1, 2)	1ν ₂₃	[72069]
	9130.13	(0.03)	4(1, 3) - 3(1, 2)	2ν ₂₃	[72069]
	9132.37	(0.02)	4(1, 3) - 3(1, 2)	1ν ₄₈	[72069]
	9134.09	(0.03)	4(1, 3) - 3(1, 2)	1ν ₂₃ 1ν ₄₈	[72069]
	9137.98	(0.03)	4(1, 3) - 3(1, 2)	2ν ₄₈	[72069]
	9404.97	(0.03)	36(11,25) - 36(11,26)	2ν ₂₃	[72069]
	9454.58	(0.02)	5(1, 5) - 4(1, 4)		[72069]
	9459.13	(0.03)	5(1, 5) - 4(1, 4)	1ν ₄₇	[72069]
	9460.85	(0.02)	5(1, 5) - 4(1, 4)	1ν ₂₃	[72069]
	9461.78	(0.02)	5(1, 5) - 4(1, 4)	1ν ₄₈	[72069]
	9465.64	(0.02)	62(19,43) - 62(19,44)		[72069]
	9467.09	(0.03)	5(1, 5) - 4(1, 4)	2ν ₂₃	[72069]
	9467.99	(0.03)	5(1, 5) - 4(1, 4)	1ν ₂₃ 1ν ₄₈	[72069]
	9468.79	(0.03)	5(1, 5) - 4(1, 4)	2ν ₄₈	[72069]
	9517.82	(0.02)	36(11,25) - 36(11,26)	1ν ₂₃	[72069]
	9631.96	(0.02)	36(11,26) - 36(11,25)		[72069]
	9661.65	(0.02)	7(1, 6) - 7(1, 7)		[72069]
	9666.31	(0.03)	36(11,25) - 36(11,26)	1ν ₄₇	[72069]
	9688.03	(0.03)	36(11,25) - 36(11,26)	1ν ₂₃ 1ν ₄₈	[72069]
	9696.44	(0.02)	5(0, 5) - 4(0, 4)		[72069]
	9700.39	(0.03)	5(0, 5) - 4(0, 4)	1ν ₄₇	[72069]
	9702.37	(0.02)	5(0, 5) - 4(0, 4)	1ν ₄₈	[72069]
	9702.88	(0.02)	5(0, 5) - 4(0, 4)	1ν ₂₃	[72069]
	9708.16	(0.03)	5(0, 5) - 4(0, 4)	2ν ₄₈	[72069]
	9708.80	(0.03)	5(0, 5) - 4(0, 4)	1ν ₂₃ 1ν ₄₈	[72069]
	9709.30	(0.03)	5(0, 5) - 4(0, 4)	2ν ₂₃	[72069]
	9777.83	(0.02)	72(22,50) - 72(22,51)		[72069]
	9781.61	(0.02)	6(2, 5) - 6(0, 6)		[72069]
	9804.38	(0.02)	36(11,25) - 36(11,26)	1ν ₄₈	[72069]
	9887.06	(0.02)	49(15,34) - 49(15,35)		[72069]
	9945.43	(0.03)	49(15,34) - 49(15,35)	1ν ₄₇	[72069]
	10055.11	(0.03)	33(10,23) - 33(10,24)	2ν ₂₃	[72069]
	10108.65	(0.02)	12(3, 9) - 12(3, 10)	1ν ₂₃	[72069]
	10140.45	(0.02)	12(3, 10) - 12(3, 9)		[72069]
	10158.93	(0.02)	12(3, 9) - 12(3, 10)	1ν ₄₈	[72069]
	10160.99	(0.02)	33(10,23) - 33(10,24)	1ν ₂₃	[72069]
	10267.81	(0.02)	33(10,24) - 33(10,23)		[72069]
	10297.24	(0.03)	33(10,23) - 33(10,24)	1ν ₄₇	[72069]
	10315.48	(0.03)	33(10,23) - 33(10,24)	1ν ₂₃ 1ν ₄₈	[72069]
	10423.95	(0.02)	33(10,33) - 33(10,24)	1ν ₄₈	[72069]
	10491.05	(0.02)	5(2, 4) - 4(2, 3)		[72069]
	10494.46	(0.03)	5(2, 4) - 4(2, 3)	1ν ₄₇	[72069]
	10494.99	(0.02)	5(2, 4) - 4(2, 3)	1ν ₂₃	[72069]

TABLE 88.3. Microwave spectrum of azulene — Continued

C₁₀H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	10498.32	(0.02)	5(2, 4) - 4(2, 3)	1ν ₄₈	[72069]
	10498.98	(0.03)	5(2, 4) - 4(2, 3)	2ν ₂₃	[72069]
	10502.27	(0.03)	5(2, 4) - 4(2, 3)	1ν ₂₃	[72069]
	10505.52	(0.03)	5(2, 4) - 4(2, 3)	2ν ₄₈	[72069]
	10558.82	(0.02)	59(18,41) - 59(18,42)		[72069]
	10707.05	(0.02)	30(9,21) - 30(9,22)	1ν ₂₃	[72069]
	10764.53	(0.02)	5(4, 2) - 4(4, 1)		[72069]
	10767.43	(0.02)	5(4, 2) - 4(4, 1)	1ν ₂₃	[72069]
	10768.65	(0.02)	5(4, 1) - 4(4, 0)		[72069]
	10770.25	(0.03)	5(4, 2) - 4(4, 1)	2ν ₂₃	[72069]
	10771.52	(0.02)	5(4, 1) - 4(4, 0)	1ν ₂₃	[72069]
	10772.78	(0.02)	5(4, 2) - 4(4, 1)	1ν ₄₈	[72069]
	10774.40	(0.03)	5(4, 1) - 4(4, 0)	2ν ₂₃	[72069]
	10775.58	(0.03)	5(4, 2) - 4(4, 1)	1ν ₂₃	[72069]
	10776.94	(0.02)	5(4, 1) - 4(4, 0)	1ν ₄₈	[72069]
	10779.75	(0.03)	5(4, 1) - 4(4, 0)	1ν ₂₃	[72069]
	10780.84	(0.03)	5(4, 2) - 4(4, 1)	2ν ₄₈	[72069]
	10782.18	(0.02)	5(3, 3) - 4(3, 2)		[72069]
	10785.07	(0.02)	5(3, 3) - 4(3, 2)	1ν ₂₃	[72069]
	10785.09	(0.03)	5(4, 1) - 4(4, 0)	2ν ₄₈	[72069]
	10785.44	(0.03)	5(3, 3) - 4(3, 2)	1ν ₄₇	[72069]
	10787.99	(0.03)	5(3, 3) - 4(3, 2)	2ν ₂₃	[72069]
	10790.29	(0.02)	5(3, 3) - 4(3, 2)	1ν ₄₈	[72069]
	10793.16	(0.03)	5(3, 3) - 4(3, 2)	1ν ₂₃	[72069]
	10794.51	(0.03)	15(4,11) - 15(4,12)	2ν ₂₃	[72069]
	10798.30	(0.03)	5(3, 3) - 4(3, 2)	2ν ₄₈	[72069]
	10804.88	(0.02)	30(9,22) - 30(9,21)		[72069]
	10823.51	(0.02)	46(14,32) - 46(14,33)		[72069]
	10828.71	(0.03)	30(9,21) - 30(9,22)	1ν ₄₇	[72069]
	10836.47	(0.02)	15(4,11) - 15(4,12)	1ν ₂₃	[72069]
	10843.06	(0.03)	30(9,21) - 30(9,22)	1ν ₂₃	[72069]
	10870.77	(0.03)	15(4,11) - 15(4,12)	1ν ₂₃	[72069]
	10875.31	(0.03)	15(4,11) - 15(4,12)	1ν ₄₇	[72069]
	10878.53	(0.02)	15(4,12) - 15(4,11)		[72069]
	10906.95	(0.02)	5(3, 2) - 4(3, 1)		[72069]
	10909.15	(0.02)	5(3, 2) - 4(3, 1)	1ν ₂₃	[72069]
	10910.30	(0.03)	5(3, 2) - 4(3, 1)	1ν ₄₇	[72069]
	10911.34	(0.03)	5(3, 2) - 4(3, 1)	2ν ₂₃	[72069]
	10912.90	(0.02)	15(4,11) - 15(4,12)	1ν ₄₈	[72069]
	10915.87	(0.02)	5(3, 2) - 4(3, 1)	1ν ₄₈	[72069]
	10918.06	(0.03)	5(3, 2) - 4(3, 1)	1ν ₂₃	[72069]
	10924.71	(0.03)	5(3, 2) - 4(3, 1)	2ν ₄₈	[72069]
	10942.08	(0.02)	30(9,21) - 30(9,22)	1ν ₄₈	[72069]
	10989.35	(0.02)	69(21,48) - 69(21,49)		[72069]
	11036.67	(0.03)	27(8,19) - 27(8,20)	2ν ₂₃	[72069]
	11080.73	(0.03)	30(9,21) - 30(9,22)	2ν ₄₈	[72069]
	11123.58	(0.02)	27(8,19) - 27(8,20)	1ν ₂₃	[72069]
	11211.10	(0.02)	27(8,20) - 27(8,19)		[72069]
	11214.17	(0.03)	18(5,13) - 18(5,14)	2ν ₂₃	[72069]
	11216.86	(0.02)	79(24,55) - 79(24,56)		[72069]
	11229.03	(0.03)	27(8,19) - 27(8,20)	1ν ₄₇	[72069]
	11239.21	(0.03)	27(8,19) - 27(8,20)	1ν ₂₃	[72069]
	11250.41	(0.02)	5(1, 4) - 4(1, 3)		[72069]
	11251.66	(0.02)	6(1, 6) - 5(1, 5)		[72069]
	11253.22	(0.02)	5(1, 4) - 4(1, 3)	1ν ₂₃	[72069]
	11256.06	(0.03)	5(1, 4) - 4(1, 3)	2ν ₂₃	[72069]
	11256.83	(0.02)	5(1, 4) - 4(1, 3)	1ν ₄₈	[72069]
	11257.21	(0.03)	6(1, 6) - 5(1, 5)	1ν ₄₇	[72069]
	11259.43	(0.02)	6(1, 6) - 5(1, 5)	1ν ₂₁	[72069]
	11260.15	(0.02)	6(1, 6) - 5(1, 5)	1ν ₄₈	[72069]
	11263.17	(0.03)	5(1, 4) - 4(1, 3)	2ν ₄₈	[72069]
	11267.18	(0.02)	18(5,13) - 18(5,14)	1ν ₂₃	[72069]
	11267.90	(0.03)	6(1, 6) - 5(1, 5)	1ν ₂₃	[72069]
	11268.42	(0.03)	6(1, 6) - 5(1, 5)	2ν ₄₈	[72069]
	11301.78	(0.03)	24(7,17) - 24(7,18)	2ν ₂₃	[72069]
	11319.93	(0.03)	18(5,13) - 18(5,14)	1ν ₂₃	[72069]
	11320.36	(0.02)	18(5,14) - 18(5,13)		[72069]

TABLE 88.3. Microwave spectrum of azulene — Continued

C₁₀H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
	11321.46	(0.03)	18(5,13) - 18(5,14)	1ν ₄₇	[72069]
	11327.58	(0.02)	27(8,19) - 27(8,20)	1ν ₄₈	[72069]
	11355.60	(0.02)	10(2, 8) - 10(2, 9)	1ν ₂₃	[72069]
	11372.00	(0.03)	21(6,15) - 21(6,16)	2ν ₂₃	[72069]
	11373.26	(0.02)	18(5,13) - 18(5,14)	1ν ₄₈	[72069]
	11377.70	(0.02)	24(7,17) - 24(4,18)	1ν ₂₃	[72069]
	11381.31	(0.02)	10(2, 8) - 10(2, 9)		[72069]
	11383.83	(0.02)	10(2, 8) - 10(2, 9)	1ν ₄₈	[72069]
	11400.52	(0.02)	6(0, 6) - 5(0, 5)		[72069]
	11405.61	(0.03)	6(0, 6) - 5(0, 5)	1ν ₄₇	[72069]
	11407.93	(0.02)	6(0, 6) - 5(0, 5)	1ν ₄₈	[72069]
	11408.58	(0.02)	6(0, 6) - 5(0, 5)	1ν ₂₃	[72069]
	11416.59	(0.03)	6(0, 6) - 5(0, 5)	2ν ₂₃	[72069]
	11418.16	(0.02)	5(2, 3) - 4(2, 2)		[72069]
	11419.17	(0.02)	5(2, 3) - 4(2, 2)	1ν ₂₃	[72069]
	11420.19	(0.03)	5(2, 3) - 4(2, 2)	2ν ₂₃	[72069]
	11421.00	(0.03)	5(2, 3) - 4(2, 2)	1ν ₄₇	[72069]
	11426.47	(0.03)	18(5,13) - 18(5,14)	2ν ₄₈	[72069]
	11427.25	(0.02)	5(2, 3) - 4(2, 2)	1ν ₄₈	[72069]
	11428.25	(0.03)	5(2, 3) - 4(2, 2)	1ν ₂₃	1ν ₄₈ [72069]
	11436.31	(0.03)	5(2, 3) - 4(2, 2)	2ν ₄₈	[72069]
	11436.45	(0.02)	21(6,15) - 21(6,16)	1ν ₂₃	[72069]
	11444.90	(0.03)	27(8,19) - 27(8,20)	2ν ₄₈	[72069]
	11454.04	(0.02)	24(7,18) - 24(7,17)		[72069]
	11466.00	(0.03)	24(7,17) - 24(7,18)	1ν ₄₇	[72069]
	11472.01	(0.03)	24(7,17) - 24(7,18)	1ν ₂₃	1ν ₄₈ [72069]
	11501.20	(0.02)	21(6,16) - 21(6,15)		[72069]
	11507.50	(0.03)	21(6,15) - 21(6,16)	1ν ₄₇	[72069]
	11509.54	(0.03)	21(6,15) - 21(6,16)	1ν ₂₃	1ν ₄₈ [72069]
	11548.89	(0.02)	24(7,17) - 24(7,18)	1ν ₄₈	[72069]
	11574.56	(0.02)	21(6,15) - 21(6,16)	1ν ₄₈	[72069]
	11575.66	(0.02)	43(13,30) - 43(13,31)	1ν ₂₃	[72069]
	11644.27	(0.03)	24(7,17) - 24(7,18)	2ν ₄₈	[72069]
	11648.29	(0.03)	21(6,15) - 21(6,16)	2ν ₄₈	[72069]
	11681.98	(0.02)	56(17,39) - 56(17,40)		[72069]
	11731.54	(0.02)	43(13,30) - 43(13,31)		[72069]
	11781.89	(0.03)	43(13,30) - 43(13,31)	1ν ₄₇	[72069]
	12219.29	(0.02)	8(3, 6) - 8(1, 7)		[72069]
	12259.73	(0.02)	66(20,46) - 66(20,47)		[72069]
	12434.19	(0.02)	40(12,28) - 40(12,29)	1ν ₂₃	[72069]
	12480.69	(0.02)	6(2, 5) - 5(2, 4)		[72069]
	12582.42	(0.02)	40(12,28) - 40(12,29)		[72069]

Table 89.1. Molecular constants for bullvalene. [76061]

Vibrational State	B_V (MHz)	q_V (MHz)	E (cm^{-1})
Ground	1644.304(8)		0
$\nu_a = 1$	1644.822(8)	0.557	248(10)
$\nu_b = 1$	1644.970(8)		266(10)
$\nu_c = 1$	1644.163		373(10)
$\nu_d = 1$	1644.754		447(10)
$\nu_e = 1$	1645.142		574(10)
$\nu_a = 2$	1645.328		
$\nu_b = 2$	1645.630		
$\nu_c = 2$	1644.031		
$\nu_a = 3$	1645.825		
$\nu_b = 3$	1646.290		

TABLE 89.2. Microwave spectrum of bullvalene

C₁₀H₁₀


Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' - J''$	Vib. state	Ref.
C ₁₀ H ₁₀ BULLVALENE 	9865.89	(0.01)	3 - 2		[75059]
	19728.48	(0.03)	6 - 5	2ν c	[76061]
	19730.04	(0.03)	6 - 5	1ν c	[76061]
	19731.73	(0.03)	6 - 5		[76061]
	19737.96	(0.03)	6 - 5	1ν a	[76061]
	19739.73	(0.03)	6 - 5	1ν b	[76061]
	19744.03	(0.03)	6 - 5	2ν a	[76061]
	19745.87	(0.03)	6 - 5	1ν a	1ν b [76061]
	19747.64	(0.03)	6 - 5	2ν b	[76061]
	23016.53	(0.03)	7 - 6	2ν c	[76061]
	23018.37	(0.03)	7 - 6	1ν c	[76061]
	23020.33	(0.03)	7 - 6		[76061]
	23027.58	(0.03)	7 - 6	1ν a	[76061]
	23029.65	(0.03)	7 - 6	1ν b	[76061]
	23034.68	(0.03)	7 - 6	2ν a	[76061]
	23036.83	(0.03)	7 - 6	1ν a	1ν b [76061]
	23038.92	(0.03)	7 - 6	2ν b	[76061]
	23052.99	(0.03)	7 - 6	2ν a	2ν b [76061]
	26304.54	(0.03)	8 - 7	2ν c	[76061]
	26306.67	(0.03)	8 - 7	1ν c	[76061]
	26308.92	(0.03)	8 - 7		[76061]
	26317.20	(0.03)	8 - 7	1ν a	[76061]
	26319.58	(0.03)	8 - 7	1ν b	[76061]
	26325.30	(0.03)	8 - 7	2ν a	[76061]
	26327.77	(0.03)	8 - 7	1ν a	1ν b [76061]
	26330.17	(0.03)	8 - 7	2ν b	[76061]
	26346.21	(0.03)	8 - 7	2ν a	2ν b [76061]
	29592.49	(0.03)	9 - 8	2ν c	[76061]
	29594.91	(0.03)	9 - 8	1ν c	[76061]
	29597.48	(0.01)	9 - 8		[75059]
	29603.96	(0.03)	9 - 8	1ν a	1ν c [76061]
	29605.65	(0.03)	9 - 8	1ν d	[76061]
	29606.82	(0.03)	9 - 8	1ν a	[76061]
	29609.47	(0.03)	9 - 8	1ν b	[76061]
	29612.62	(0.03)	9 - 8	1ν e	[76061]
	29615.92	(0.03)	9 - 8	2ν a	[76061]
	29618.75	(0.03)	9 - 8	1ν a	1ν b [76061]
	29621.32	(0.03)	9 - 8	2ν b	[76061]
	29625.10	(0.03)	9 - 8	3ν a	[76061]
	29627.65	(0.03)	9 - 8	2ν a	1ν b [76061]
	32880.60	(0.03)	9 - 8	2ν c	[76061]
	32883.25	(0.03)	9 - 8	1ν c	[76061]
	32885.99	(0.01)	10 - 9		[75059]
	32890.82	(0.03)	10 - 9	1ν a	ℓ = l ₁ [76061]
	32893.24	(0.03)	10 - 9	1ν a	1ν c [76061]
	32895.06	(0.03)	10 - 9	1ν d	[76061]
	32896.38	(0.03)	10 - 9	1ν a	[76061]
	32899.36	(0.03)	10 - 9	1ν b	[76061]
	32901.98	(0.03)	10 - 9	1ν a	ℓ = u ₁ [76061]
	32902.87	(0.03)	10 - 9	1ν e	[76061]
	32906.51	(0.03)	10 - 9	2ν a	[76061]
	32908.35	(0.03)	10 - 9	1ν b	1ν d [76061]
	32909.62	(0.03)	10 - 9	1ν a	1ν b [76061]
	32912.65	(0.03)	10 - 9	2ν b	[76061]
	32916.50	(0.03)	10 - 9	3ν a	[76061]
	32919.65	(0.03)	10 - 9	2ν a	1ν b [76061]
	32922.80	(0.03)	10 - 9	1ν a	2ν b [76061]
32926.00	(0.03)	10 - 9	3ν b	[76061]	
36168.60	(0.03)	11 - 10	2ν c	[76061]	
36171.45	(0.03)	11 - 10	1ν c	[76061]	
36174.55	(0.01)	11 - 10		[75059]	
36179.76	(0.03)	11 - 10	1ν a	ℓ = l ₁ [76061]	
36182.50	(0.03)	11 - 10	1ν a	1ν c [76061]	
36184.70	(0.03)	11 - 10	1ν d	[76061]	
36185.95	(0.03)	11 - 10	1ν a	[76061]	
36189.24	(0.03)	11 - 10	1ν b	[76061]	
36192.00	(0.03)	11 - 10	1ν a	ℓ = u ₁ [76061]	
36193.06	(0.03)	11 - 10	1ν e	[76061]	

TABLE 89.2. Microwave spectrum of bullvalene — Continued

C₁₀H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J' - J''$	Vib. state	Ref.
	36197.10	(0.03)	11 - 10	2v a	[76061]
	36199.28	(0.03)	11 - 10	1v b	[76061]
	36200.42	(0.03)	11 - 10	1v a	[76061]
	36203.72	(0.03)	11 - 10	2v b	[76061]
	36208.02	(0.03)	11 - 10	3v a	[76061]
	36211.52	(0.03)	11 - 10	2v a	[76061]
	36214.88	(0.03)	11 - 10	1v a	[76061]
	36225.92	(0.03)	11 - 10	2v a	[76061]
	39456.51	(0.01)	12 - 11	2v c	[76061]
	39459.69	(0.01)	12 - 11	1v c	[76061]
	39463.05	(0.01)	12 - 11		[75059]
	39468.74	(0.03)	12 - 11	1v a	[76061]
	39471.83	(0.01)	12 - 11	1v a	[76061]
	39473.93	(0.01)	12 - 11	1v d	[76061]
	39475.48	(0.01)	12 - 11	1v a	[76061]
	39479.06	(0.01)	12 - 11	1v b	[76061]
	39482.10	(0.01)	12 - 11	1v a	[76061]
	39483.32	(0.01)	12 - 11	1v e	[76061]
	39487.68	(0.01)	12 - 11	2v a	[76061]
	39490.00	(0.01)	12 - 11	1v b	[76061]
	39491.35	(0.01)	12 - 11	1v a	[76061]
	39494.94	(0.01)	12 - 11	2v b	[76061]
	39499.60	(0.01)	12 - 11	3v a	[76061]
	39503.38	(0.01)	12 - 11	2v a	[76061]
	39507.12	(0.01)	12 - 11	1v a	[76061]
	39510.70	(0.01)	12 - 11	3v b	[76061]
	39519.01	(0.01)	12 - 11	2v a	[76061]

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