

Microwave Spectral Tables. III. Hydrocarbons, CH to C₁₀H₁₀

F. J. Lovas and R. D. Suenram

National Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, MD 20899

Received May 26, 1988; revised manuscript received October 29, 1988

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.

CONTENTS

1. Introduction	1250	CH ₂		
1.1. General Description of the Tables	1250	2.1. Molecular parameters of CH ₂ (X ³ B ₁) ...	1258	
1.1.a. Molecular Constant Tables	1250	2.2. Molecular parameters of ¹³ CH ₂	1259	
1.1.b. Spectral Line Tables	1250	2.3. Molecular parameters for the (000) and (010) vibrational levels of CD ₂ in its X ³ B ₁ ground electronic state	1260	
1.2. Molecular Parameters and Energy	1250	2.4. Microwave spectrum of methylene radical	1261	
1.2.a. Linear Molecules	1250			
1.2.b. Symmetric Top Molecules	1251	CH ₄		
1.2.c. Asymmetric Top Molecules	1251	3.1. Molecular constants for CH ₄ and ¹³ CH ₄	1262	
1.2.d. Molecules with Doublet Electronic Ground States	1253	3.2. Molecular constants for CH ₃ D and CH ₂ D ₂	1262	
1.3. Evaluation of the Spectral Data	1253	3.3. Molecular constants for CD ₄ and ¹³ CH ₄	1262	
1.3.a. General Procedure	1253	3.4. Microwave spectrum of methane	1263	
1.4. List of Symbols	1253	C ₂ H		
1.4.a. Quantum Numbers	1253	4.1. Molecular constants for the ethynyl radical	1265	
1.4.b. Molecular Constants	1254	4.2. Microwave spectrum of ethynyl radical	1266	
1.5. Special Units, Fundamental Constants and Useful Conversion Factors	1254	C ₂ H ₂		
1.5.a. Special Units	1254	5.1. Molecular constants for d ₁ -acetylene (HCCD)	1267	
1.5.b. Fundamental Constants and Conversion Factors	1255	5.2. Molecular constants for DCCD from the ν ₅ ¹ - ν ₄ ¹ band	1267	
1.6. Acknowledgments	1255	5.3. Microwave spectrum of acetylene (C ₂ H ₂)	1268	
1.7. References to the Introduction	1255	C ₂ H ₄		
2. Molecular Constants and Spectral Line Tables (see List of Tables below)	1255	6.1. Molecular constants for deuterated ethylene	1268	
3. References to Spectral Data	1521	6.2. Microwave spectrum of ethylene	1269	
		C ₂ H ₆		
		7.1. Molecular constants for ¹² C and ¹³ C isotopic forms of CH ₃ CD ₃	1270	
		7.2. Molecular constants for CH ₃ CHD ₂	1270	
		7.3. Molecular constants of CH ₃ CH ₂ D, CD ₃ CH ₂ D and <i>gauche</i> -CH ₂ DCH ₂ D	1271	

List of Tables

CH

1.1. Molecular constants for ¹² CH and ¹³ CH	1256
1.2. Microwave spectrum of methylidyne radical	1257

©1989 by the U. S. Secretary of Commerce on behalf of the United States. This copyright is assigned to the American Institute of Physics and the American Chemical Society.

Reprints available from ACS; see Reprints List at back of issue.

7.4.	Microwave spectrum of ethane	1272	C_3H_8	14.1.	Molecular constants for propane	1210
C_3H				14.2.	Rotational constants and electric dipole moment for ^{13}C and deuterated isotopic species of propane	1311
8.1.	Molecular constants of CCCH in the $X^2\Pi$ state	1276		14.3.	Microwave spectrum of propane	1312
8.2.	Molecular constants of the c - C_3H radical	1276	C_4H	15.1.	Molecular constants for the C_4H radical	1216
8.3.	Microwave spectrum of ℓ - C_3H radical	1277		15.2.	Microwave spectrum of butadiynyl radical	1317
8.4.	Microwave spectrum of cyclic- C_3H radical	1278	C_4H_2	16.1.	Molecular constants of 1,3-butadiyne (diacetylene) in excited vibrational states	1318
C_3H_2				16.2.	Molecular constants of $HC\equiv CC\equiv CD$	1319
9.1.	Molecular constants for cyclopropenyli-dene (HCCCH)	1279		16.3.	Molecular constants of diacetylene- d_2 in excited vibrational states	1319
9.2.	Molecular constants for cyclopropenyli-dene and its monosubstituted deriva-tives	1280		16.4.	Microwave spectrum of 1,3-butadiyne ..	1320
9.3.	Microwave spectrum of cyclopropenyli-dene	1281	C_4H_4	17.1.	Rotational constants for the ground, the $\nu_{13} = 1$ and the $\nu_{18} = 1$ states of 1-bu-tene-3-yne-4d	1325
C_3H_4				17.2.	Rotational analysis for the ground state of 1-butene-3-yne in the present work...	1325
10.1.	Molecular constants for allene in vibra-tionally excited states	1288		17.3.	Microwave spectrum of 1-butene-3-yne	1326
10.2.	Molecular constants for allene- d_1 and allene-1,1- d_2	1288		18.1.	Molecular constants for methylene cy-clopropene and its ^{13}C isotopic forms ...	1328
10.3.	Microwave spectrum of allene	1289		18.2.	Microwave spectrum of methylenecy-clopropene	1329
11.1.	Molecular constants for cyclopropene and 1,2-dideuterocyclopropene	1290	C_4H_6	19.1.	Molecular constants for 2-butyne1,1,1- d_3	1329
11.2.	Rotational constants for $^{13}C_1$, $^{13}C_2$, D_2 (methylene) and D (ethylene) species of cyclopropene	1290		19.2.	Microwave spectrum of 2-butyne1,1,1- d_3	1330
11.3.	Microwave spectrum of cyclopropene	1290		20.1.	Molecular constants for 1-butyne (C_4H_6) in the ground and lowest tor-sional and bending states	1333
12.1.	Molecular constants for propyne and ^{13}C -propyne in the ground vibra-tional state	1295		20.2.	Molecular constants for the vibrationally excited states $\nu_{15} = 2$ and 3 and $\nu_{14} = 1$ of 1-butyne	1334
12.2.	Molecular constants for deuterated spe-cies of CH_3CCH	1296		20.3.	Microwave spectrum of 1-butyne	1335
12.3.	Molecular constants for propyne in the $\nu_9 = 1$ and $\nu_5 = 1$ vibrational state	1296		21.1.	Molecular constants for 1,2-butadiene (methylallene)	1343
12.4.	Molecular constants for propyne in the ν_{10} excited state	1297		21.2.	Microwave spectrum of methylallene. ..	1344
12.5.	Microwave spectrum of propyne	1297		22.1.	Molecular constants for bicyclo-[1.1.0]butane	1345
C_3H_6				22.2.	Microwave spectrum of bicyclo-[1.1.0]butane	1346
13.1.	Molecular constants for the ground state of propylene from fitting internal rota-tion and the A state alone	1304		23.1.	Molecular constants for cyclobutene and its ^{13}C isotopic species	1347
13.2.	Dipole moment and Zeeman constants for propylene	1304		23.2.	Molecular constants for monodeutero-species of cyclobutene	1347
13.3.	Molecular constants for propylene ($CH_3CH=CH_2$) in excited torsional states	1304		23.3.	Microwave spectrum of cyclobutene	1348
13.4.	Molecular constants for the deuterated propylene species t - $CHDCHCH_3$ and CH_2CDCH_3 in the ground and excited torsional states	1305		24.1.	Molecular constants for 1-methylcyclo-pene	1351
13.5.	Rotational constants for substituted iso-topic forms of propylene	1305		24.2.	Microwave spectrum of methylcyclo-pene	1352
13.6.	Microwave spectrum of propylene	1306		25.1.	Molecular constants for methylenecy-clopropane	1353
13.1.a.	Molecular constants for cyclopropane-1,1- d_2	1308				
13.2.a.	Microwave spectrum of cyclopropane ..	1309				

25.2.	Rotational constants for the ^{13}C isotop species of methylenecyclopropane	1353	33.3.	Microwave spectrum of methyl diacetylene	1382
25.3.	Microwave spectrum of methylenecyclopropane	1354			
C_4H_8			C_5H_6		
26.1.	Molecular constants for the ground vibrational state of <i>cis</i> - and <i>skew</i> -1-butene	1355	34.1.	Molecular constants for cyclopentadiene	1385
26.2.	Molecular constants for excited vibrational states of 1-butene	1355	34.2.	Rotational constants for ^{13}C substituted cyclopentadiene	1385
26.3.	Rotational constants for deuterated and ^{13}C isotopic forms of 1-butene	1356	34.3.	Microwave spectrum of cyclopentadiene	1386
26.4.	Centrifugal distortion constants for isotopic forms of 1-butene	1357	35.1.	Molecular constants for 1-penten-3-yne	1387
26.5.	Microwave spectrum of 1-butene	1358	35.2.	Microwave spectrum of 1-penten-3-yne	1387
27.1.	Molecular constants for <i>cis</i> -2-butene in the ground state	1364	36.1.	Rotational constants and dipole moment for normal and deuterated cyclopropylacetylene	1387
27.2.	Molecular constants for <i>sym</i> - $\text{CH}_2\text{DCHCHCH}_3$, <i>asy</i> - $\text{CH}_2\text{DCHCHCH}_3$ and $\text{CH}_3\text{CDCDCH}_3$	1365	36.2.	Rotational constants for ^{13}C isotopic forms of cyclopropylacetylene	1387
27.3.	Molecular constants for $\text{CH}_3\text{CDCHCH}_3$	1366	36.3.	Microwave spectrum of cyclopropylacetylene	1388
27.4.	Molecular constants for d_8 <i>cis</i> -2-butene and d_6 <i>cis</i> -2-butene	1366	37.1.	Molecular constants for 2-methyl-1-buten-3-yne	1389
27.5.	Microwave spectrum of <i>cis</i> -2-butene	1367	37.2.	Microwave spectrum of 2-methyl-1-buten-3-yne	1390
28.1.	Molecular constants for isobutylene (2-methyl-propene) in the ground and torsionally excited states	1370	38.1.	Molecular constants for <i>cis</i> -3-penten-1-yne	1391
28.2.	Rotational analysis of isobutylene AA state from the present study	1370	38.2.	Microwave spectrum of <i>cis</i> -3-penten-1-yne	1391
28.3.	Rotational constants for deuterated and ^{13}C isotopic species of isobutylene	1370	39.1.	Molecular constants for bicyclo-[2.1.0]pent-2-ene	1392
28.4.	Microwave spectrum of isobutylene	1371	39.2.	Microwave spectrum of bicyclo-[2.1.0]pent-2-ene	1392
29.1.	Molecular constants for methylcyclopropane	1373	39.1.a.	Molecular constants for 1,2,3-pentatriene	1392
29.2.	Microwave spectrum of methylcyclopropane	1374	39.2.a.	Microwave spectrum of 1,2,3-pentatriene	1393
29.1.a.	Molecular constants for cyclobutane- d_1	1374			
29.2.a.	Microwave spectrum of cyclobutane- d_1	1375	C_5H_8		
C_4H_{10}			40.1.	Molecular constants for <i>trans</i> -isoprene (2-methyl-1,3-butadiene)	1394
30.1.	Molecular constants for the isobutane species: $(\text{CH}_3)_3\text{CH}$, $(\text{CH}_3)_3^{13}\text{CH}$ and $(\text{CH}_3)_3\text{CD}$	1376	40.2.	Microwave spectrum of isoprene	1395
30.2.	Rotational constants for asymmetric rotor species of isobutane	1376	41.1.	Molecular constants for 3-methyl-1-butyne (isopropyl acetylene)	1396
30.3.	Microwave spectrum of isobutane	1376	41.2.	Rotational constants for the excited vibrational states and isotopic species of 3-methyl-1-butyne	1396
31.1.	Molecular constants for the C_5H radical	1377	41.3.	Microwave spectrum of 3-methyl-1-butyne	1397
31.2.	Microwave spectrum of C_5H	1377	42.1.	Molecular constants for the ground vibrational state of <i>trans</i> - and <i>gauche</i> -1-pentyne	1399
C_5H_4			42.2.	Molecular constants for excited vibrational states of <i>trans</i> - and <i>gauche</i> -1-pentyne	1400
32.1.	Rotational and centrifugal distortion constants for 1,4-pentadiyne	1378	42.3.	Microwave spectrum of 1-pentyne	
32.2.	Microwave spectrum of 1,4-pentadiyne	1379	43.1.	Molecular constants of <i>trans</i> -vinyl cyclopropane	1401
33.1.	Molecular constants for 1,3-pentadiyne and deuterated isotopic species in the ground state	1381	43.2.	Microwave spectrum of vinyl cyclopropane	1407
33.2.	Rotational constants for 1,3-pentadiyne in the first excited vibrational state ($\nu = 1$) and for various ^{13}C substituted forms in the ground state	1381	44.1.	Molecular constants for methylene cyclobutane	1408

44.2.	Microwave spectrum of methylene cyclobutane	1409	56.4.	Microwave spectrum of 3,4-dimethylenecyclobutene	1443
45.1.	Molecular constants for 1-methyl cyclobutene	1411	57.1.	Molecular constants of tricyclo[3.1.0.0 ^{2,6}]hex-3-ene (benzvalene) ..	1446
45.2.	Microwave spectrum of 1-methyl cyclobutene	1412	57.2.	Microwave spectrum of tricyclo[3.1.0.0 ^{2,6}]hex-3-ene	1447
46.1.	Molecular constants for 1,1-dimethylallene in the ground vibrational state	1414	58.1.	Molecular constants of 1-methylene-2,4-cyclopentadiene (fulvene)	1448
46.2.	Rotational constants for excited vibrational states of 1,1-dimethylallene	1414	58.2.	Microwave spectrum of 1-methylene-2,4-cyclopentadiene	1449
46.3.	Microwave spectrum of dimethylallene .	1415	59.1.	Molecular constants of bicyclo[2.2.0]hexa-2,5-diene (dewar benzene)	1450
47.1.	Molecular constants for <i>trans</i> - and <i>cis</i> -1,1-pentadiene	1420	59.2.	Microwave spectrum of bicyclo[2.2.0]hexa-2,5-diene	1451
47.2.	Microwave spectrum of 1,3-pentadiene	1421	60.1.	Molecular constants for benzene-d ₁	1451
48.1.	Molecular constants for bicyclo[2.1.0]pentane	1422	60.2.	Microwave spectrum of benzene-d	1452
48.2.	Microwave spectrum of bicyclo[2.1.0]pentane	1423			
49.1.	Molecular constants of 3,3-dimethylcyclopropene	1424	C₆H₈		
49.2.	Microwave spectrum of 3,3-dimethylcyclopropene	1424	61.1.	Molecular constants 1,3-cyclohexadiene	1453
50.1.	Molecular constants for cyclopentene in the ground state and excited out-of-plane bending state	1425	61.2.	Microwave spectrum of 1,3-cyclohexadiene	1453
50.2.	Microwave spectrum of cyclopentene ...	1426	62.1.	Molecular constants for tricyclo[2.2.0.0 ^{2,6}]hexane	1454
C₅H₁₀			62.2.	Microwave spectrum of tricyclo[2.2.0.0 ^{2,6}]hexane	1455
51.1.	Molecular constants of 1,1-dimethylcyclopropane	1429	63.1.	Molecular constants of bicyclo[2.1.1]hex-2-ene	1456
51.2.	Microwave spectrum of 1,1-dimethylcyclopropane	1430	63.2.	Microwave spectrum of bicyclo[2.1.1]hex-2-ene	1457
52.1.	Molecular constants of the ground state of <i>trans</i> -3-methyl-1-butene	1430	64.1.	Molecular constants of bicyclo[3.1.0]hex-2-ene	1458
52.2.	Molecular constants of the vibrational states of <i>trans</i> -3-methyl-1-butene	1431	64.2.	Microwave spectrum of bicyclo[3.1.0]hex-2-ene	1459
52.3.	Molecular constants for <i>gauche</i> -3-methyl-1-butene	1431	65.1.	Molecular constants of 1,2-dimethylene cyclobutane	1460
52.4.	Microwave spectrum of 3-methyl-1-butene	1432	65.2.	Molecular constants of vibrational states of 1,2-dimethylene cyclobutane ...	1460
53.1.	Molecular parameters of <i>cis</i> -2-pentene .	1434	65.3.	Microwave spectrum of 1,2-dimethylene cyclobutane	1461
53.2.	Molecular parameters of excited torsional states of <i>cis</i> -2-pentene	1435			
53.3.	Microwave spectrum of <i>cis</i> -2-pentene ...	1436	C₆H₁₀		
C₆H			66.1.	Molecular constants for <i>t</i> -butyl acetylene	1462
54.1.	Molecular constants for the C ₆ H radical in the ² Π _i state	1439	66.2.	Microwave spectrum of <i>tertiary</i> butyl acetylene	1463
54.2.	Microwave spectrum of C ₆ H radical	1440	67.1.	Molecular constants of cyclohexene	1464
C₆H₄			67.2.	Microwave spectrum of cyclohexene	1465
55.1.	Molecular constants for <i>o</i> -benzyne	1441	68.1.	Molecular constants of <i>endo</i> - and <i>exo</i> -2-methylbicyclo[2.1.0]pentane	1466
55.2.	Microwave spectrum of benzyne	1441	68.2.	Microwave spectrum of 2-methylbicyclo[2.1.0]pentane	1466
C₆H₆			69.1.	Molecular constants of methylenecyclopentane	1467
56.1.	Molecular constants for 3,4-dimethylenecyclobutene, CH = CHC(CH ₂)C(=CH ₂)	1442	69.2.	Microwave spectrum of methylenecyclopentane	1468
56.2.	Molecular constants for the ¹³ C substituted species of 3,4-dimethylenecyclobutene	1442	70.1.	Molecular constants of bicyclo[3.1.0]hexane	1469
56.3.	Molecular constants for the deuterated isotopes of 3,4-dimethylenecyclobutene	1442	70.2.	Microwave spectrum of bicyclo[3.1.0]hexane	1469

C_7H_4		80.1.	Molecular constants for methylene cyclohexane.....	1494
71.1.	Molecular constants for 1,3,5-heptatriyne (CH_3C_6H)	80.2.	Microwave spectrum of methylene cyclohexane.....	1495
71.2.	Microwave spectrum of 1,3,5-heptatriyne	C_8H_6		
C_7H_8		81.1.	Molecular constants of phenylacetylene	1496
72.1.	Molecular constants of 1,3,5-cycloheptatriene	81.2.	Molecular constants for some isotopically substituted species of phenylacetylene	1496
72.2.	Microwave spectrum of 1,3,5-cycloheptatriene	81.3.	Microwave spectrum of phenylacetylene	1497
73.1.	Molecular constants for toluene	C_8H_8		
73.2.	Microwave spectrum of toluene	82.1.	Molecular constants of methylene cycloheptatriene (heptafulvene)	1499
74.1.	Molecular constants of the ground state of spiro[2.4]hepta-4,6-diene	82.2.	Microwave spectrum of methylene cycloheptatriene	1500
74.2.	Molecular constants of some isotopically substituted species of spiro[2.4]hepta-4,6-diene	C_8H_{10}		
74.3.	Microwave spectrum of spiro[2.4]hepta-4,6-diene	83.1.	Rotational constants for <i>o</i> -xylene	1501
C_7H_{10}		83.2.	Microwave spectrum of <i>ortho</i> -xylene ...	1502
75.1.	Molecular constants of bicyclo[2.2.1]hept-2-ene (norbornene)	84.1.	Molecular constants of bicyclo[2.2.2]octadiene	1508
75.2.	Microwave spectrum of bicyclo[2.2.1]hept-2-ene	84.2.	Microwave spectrum of bicyclo[2.2.2]octadiene	1509
76.1.	Molecular constants of the ground state of 1,3-cycloheptadiene.....	C_8H_{12}		
76.2.	Molecular constants of the vibrational states of 1,3-cycloheptadiene	85.1.	Molecular constants of bicyclo[2.2.2]octene	1510
76.3.	Microwave spectrum of 1,3-cycloheptadiene	85.2.	Microwave spectrum of bicyclo[2.2.2]octene	1510
77.1.	Molecular constants of the ground state of Δ^6 -bicyclo[3.2.0]heptene	86.1.	Molecular constants of <i>axial</i> and <i>equatorial</i> ethynyl cyclohexane in the ground and lowest vibrational states	1510
77.2.	Molecular constants for the vibrational states of Δ^6 -bicyclo[3.2.0]heptene	86.2.	Microwave spectrum of ethynyl cyclohexane in the ground and lowest vibrational states	1511
77.3.	Microwave spectrum of bicyclo[3.2.0]hept-6-ene	C_9H_8		
78.1.	Molecular constants of the axial and equatorial conformers of cyclopentyl acetylene	87.1.	Molecular constants of indene	1512
78.2.	Microwave spectrum of cyclopentyl acetylene	87.2.	Microwave spectrum of indene	1512
C_7H_{12}		$C_{10}H_8$		
79.1.	Molecular constants of bicyclo[2.2.1]heptane (norbornane)	88.1.	Rotational analysis of azulene in the ground vibrational state	1513
79.2.	Microwave spectrum of bicyclo[2.2.1]heptane	88.2.	Molecular constants for azulene in the ground and excited vibrational states ...	1513
		88.3.	Microwave spectrum of azulene	1514
		$C_{10}H_{10}$		
		89.1.	Molecular constants for bullvalene	1518
		89.2.	Microwave spectrum of bullvalene	1519

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 Astronomical 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_i , 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 earlier^{4,7} 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

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

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:

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

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:

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

$$\tau_{aac} = \frac{C^2}{A^2} \tau_{aaaa} + \frac{C^2}{B^2} \tau_{aabb},$$

$$\tau_{bbc} = \frac{C^2}{B^2} \tau_{bbbb} + \frac{C^2}{A^2} \tau_{aabb},$$

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

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 workers⁸

Kivelson-Wilson parameters for planar molecules	Kirchhoff parameters (following Watson ¹⁵)	Watson parameters ¹⁶
A'	$A'' = A' - 1/2\tau'_{bbcc}$	\mathcal{A}
B'	$B'' = B' - 1/2\tau'_{aac}$	\mathcal{B}
C'	$C'' = C' - 1/2\tau'_{aabb}$	\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	
	$S = A' + B' + C'$	

⁸For 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

The authors are grateful to the many Microwave Spectroscopists who provided reprints, preprints, and data prior to publication. This review has benefited from Dr. W. H. Kirchhoff's earlier work in developing computer programs for spectral analysis and forming the spectral tables. Mrs. Gloria Rotter deserves a special acknowledgment for carrying out many of the tedious tasks involving manuscript typing, keying the spectral data, literature searching, and proofreading spectral tables.

1.7. References to the Introduction

- ¹ M.S. Cord, J.D. Peterson, M.S. Lojko, and R.H. Haas, NBS Monograph 70. Vol. IV (1968).
- ² F.J. Lovas and E. Tiemann, J. Phys. Chem. Ref. Data 3, 609 (1974).
- ³ F.J. Lovas, J. Phys. Chem. Ref. Data 7, 1445 (1978).
- ⁴ C.H. Townes and A.L. Schawlow, *Microwave Spectroscopy*, McGraw-Hill, New York, 1955.
- ⁵ W. Gordy and R.L. Cook, *Microwave Molecular Spectra in Techniques of Organic Chemistry*, Vol. IV, Pt. II, Second Ed., Interscience Publ., New York, 1970.
- ⁶ J.E. Wollrab, *Rotational Spectra and Molecular Structure*, Academic Press, New York, 1967.
- ⁷ H.W. Kroto, *Molecular Rotation Spectra*, John Wiley & Sons, New York, 1975.
- ⁸ "Report on Notation for the Spectra of Polyatomic Molecules," J. Chem. Phys. 23, 1997 (1955).
- ⁹ D.R. Lide, Jr., "Microwave Spectroscopy," in *Methods of Experimental Physics*, Vol. 3, Molecular Physics, 2d Ed., Pt. A. Academic Press, New York, 1974.

- ¹⁰ D. Kivelson and E.B. Wilson, Jr., J. Chem. Phys. 20, 1575 (1952).
- ¹¹ W.H. Kirchhoff, J. Mol. Spectrosc. 41, 333 (1972).
- ¹² H. Dreizler and G. Dendl, Z. Naturforsch. 20a, 30 (1965).
- ¹³ H. Dreizler and H.D. Rudolph, Z. Naturforsch. 20a, 749 (1965).
- ¹⁴ J.K.G. Watson, J. Chem. Phys. 45, 1360 (1966).
- ¹⁵ J.K.G. Watson, J. Chem. Phys. 48, 181 (1968).
- ¹⁶ J.K.G. Watson, J. Chem. Phys. 46, 1935 (1967).
- ¹⁷ J.K.G. Watson, J. Chem. Phys. 48, 4517 (1968).
- ¹⁸ K. Yamada and M. Winnewisser, Z. Naturforsch. 31a, 131 (1976).
- ¹⁹ G.W. King, R.M. Hainer and P.C. Cross, J. Chem. Phys. 11, 27 (1943).
- ²⁰ C.C. Lin, Phys. Rev. 116, 903 (1959).
- ²¹ J.H. Van Vleck, Rev. Modern Phys. 23, 213 (1951).
- ²² R.F. Curl, Jr. and J.L. Kinsey, J. Chem. Phys. 35, 1758 (1961).
- ²³ E.R. Cohen and B.N. Taylor, J. Phys. Chem. Ref. Data 2, 663 (1973).

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_0	843817.57(69)	843806.97 ^a
B_0	425476.852(73)	422957.033 ^a
D_0	43.8255(32)	43.303 ^a
H_0	0.0035	0.00344 ^a
Y_0	-771.11(26)	-766.5 ^a
Y_{D_0}	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
$b_F(\text{H})$	-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^1	0.0056(17)	0.504(101)
$a(^{13}\text{C})$		221.2(15)
$b_F(^{13}\text{C})$		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

CH

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]	
$^{13}\text{CH } ^2\Pi_{1/2}$		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_0 (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)			[83048]	
	1835021.	(*10.)	2(1, 1) - 2(0, 2)			[82032]	
	1892863.	(*10.)	3(1, 2) - 3(0, 3)			[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)			[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]
	μ _b (D)	0.014(5)	[75057]

TABLE 3.4. Microwave spectrum of methane

CH₄

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

TABLE 3.4. Microwave spectrum of methane — Continued

CH₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	J'	C'	T'	-	J''	C''	T''	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)					0(0, 0)				[80039]
CH ₂ D ₂	37556.666	(0.050)					1(1, 0)				[75057]
	55617.92	(0.05)					2(1, 1)				[75057]
	74188.234	(0.050)					3(2, 1)				[75057]

Table 4.1. Molecular constants for the ethynyl radical.

Parameter	CCH	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	1v ₅ c	[80037]	
	118945.132	(0.017)	2 - 1	1v ₄ c	[80037]	
	119009.24	(0.15)	2 - 1	3v ₅ c	[80037]	
	119277.553	(0.019)	2 - 1	1v ₅ d	[80037]	
	119333.134	(0.039)	2 - 1	3v ₄ c	[80037]	
	119477.295	(0.017)	2 - 1	1v ₄ d	[80037]	
	119878.22	(0.15)	2 - 1	3v ₅ d	[80037]	
	120417.362	(0.039)	2 - 1	3v ₄ d	[80037]	
	DCCD	47672.55	(0.05)	14 - 15	1v ₄ - 1v ₅ d	[77038]
		50367.48	(0.05)	14 - 15	1v ₄ - 1v ₅ c	[77038]
51084.63		(0.05)	17 - 16	1v ₅ - 1v ₄ c	[77038]	
54101.63		(0.05)	17 - 16	1v ₅ - 1v ₄ d	[77038]	
98582.83		(0.05)	13 - 14	1v ₄ - 1v ₅ d	[77038]	
101789.73		(0.05)	18 - 17	1v ₅ - 1v ₄ c	[77038]	
101113.20		(0.15)	13 - 14	1v ₄ - 1v ₅ c	[77038]	
104964.42		(0.05)	18 - 17	1v ₅ - 1v 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]
<i>c</i> -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 (u \AA^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 $I_a = 9.4965(20) \text{ u \AA}^2$.

^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±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 $\text{CH}_3\text{CH}_2\text{D}$, $\text{CD}_3\text{CH}_2\text{D}$ and gauche- $\text{CH}_2\text{DCH}_2\text{D}$. [81043]

Parameter	$\text{CH}_3\text{CH}_2\text{D}$	$\text{CD}_3\text{CH}_2\text{D}$	g- $\text{CH}_2\text{DCH}_2\text{D}$
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 CH_3CHD_2 (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)			1v ₆	[71047]
	65675.54	(0.05)	2(1, 0) - 1(1, 0)				[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]
CH ₃ ¹³ CD ₃	65006.83	(0.05)	2(1, 0) - 1(1, 0)				[77039]
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.
	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]
CH ₃ CH ₂ D	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_i	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 $X^2\Pi$ state. [86010]

Parameter	CCCH
A_{eff} (MHz)	430828.(41)
B (MHz)	11186.335(2)
$D \times 10^3$ (MHz)	5.55(2)
γ_{eff} (MHz)	36.9(11)
p (MHz)	-7.20(7)
q (MHz)	-16.62(3)
$P_D \times 10^3$ (MHz)	47.4(24)
$q_D \times 10^3$ (MHz)	1.6(6)
$P_H \times 10^6$ (MHz)	45.(6)
$q_H \times 10^6$ (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 $c\text{-C}_3\text{H}$ Radical. [87005]

Parameter	$c\text{-C}_3\text{H}$	Parameter	$c\text{-C}_3\text{H}$
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

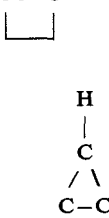
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	$F' F'_1 - F'' F''_1$	Ref.
CCHC 	91494.349	(0.030)	2(1, 2) - 1(1, 1)	5/2 3 - 3/2 2	[87005]
	91497.608	(0.030)	2(1, 2) - 1(1, 1)	5/2 2 - 3/2 2	[87005]
	91692.752	(0.030)	2(1, 2) - 1(1, 1)	3/2 1 - 1/2 0	[87005]
	91699.471	(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

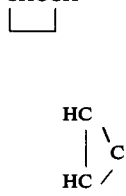
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	$F' - F''$	Ref.
CHCCH	18343.145	(0.002)	1(1, 0) - 1(0, 1)		[85018]
	46755.620	(0.020)	2(1, 1) - 2(0, 2)		[84034]
	85338.89	(0.02)	2(1, 2) - 1(0, 1)		[85019]
	118382.174	(0.020)	8(6, 3) - 8(5, 4)		[86008]
	119077.949	(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 cyclopropenyldiene — 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 CHCCH	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]
	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]

CDCCH



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		
	$\nu_{11} = 1$	$\nu_{10} = 1$	$\nu_9 = 1$
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	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)
-----------	-----------

^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]	$\begin{array}{c} \text{CH}_2 \\ / \quad \backslash \\ \text{HC}=\text{CH} \end{array}$	$\begin{array}{c} ^{13}\text{CH}_2 \\ / \quad \backslash \\ \text{HC}=\text{CH} \\ [75050] \end{array}$	$\begin{array}{c} \text{HCD} \\ / \quad \backslash \\ \text{HC}=\text{CH} \\ [75050] \end{array}$	$\begin{array}{c} \text{CH}_2 \\ / \quad \backslash \\ \text{DC}=\text{CH} \\ [59017] \end{array}$
	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.

$$B_{v_{10}} = B_0 - \alpha_{10} - q_{10} + \gamma_{11} \text{ and } B_{2v_{10}} = B_0 - 2\alpha_{10} - 4\gamma_{10}.$$

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)		$3\nu_{10} \ell = +1$	[86007]
	51698.18	(0.10)	3(0) - 2(0)		$3\nu_{10} \ell = +3$	[86007]
	51701.34	(0.10)	3(+2) - 2(+2)		$3\nu_{10} \ell = +1$	[86007]
	51701.89	(0.10)	3(+1) - 2(+1)		$3\nu_{10} \ell = +3$	[86007]
	51803.54	(0.10)	3(1) - 2(1)		$3\nu_{10} \ell = 1$	[86007]
	51804.910	(0.200)	3(-2) - 2(-2)		$4\nu_{10} \ell = +4$	[86020]
	51832.710	(0.200)	3(-1) - 2(-1)		$4\nu_{10} \ell = +2$	[86020]
	51836.464	(0.200)	3(+1) - 2(+1)		$4\nu_{10} \ell = 0$	[86020]
	51842.176	(0.200)	3(0) - 2(0)		$4\nu_{10} \ell = 0$	[86020]
	51843.421	(0.200)	3(+1) - 2(+1)		$4\nu_{10} \ell = +4$	[86020]
	51844.724	(0.200)	3(0) - 2(0)		$4\nu_{10} \ell = +2$	[86020]
	51854.655	(0.200)	3(+2) - 2(+2)		$4\nu_{10} \ell = 0$	[86020]
	51870.727	(0.200)	3(+2) - 2(+2)		$4\nu_{10} \ell = +4$	[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)		$1\nu_9 \ell = +1$	[84032]
	68384.644	(0.050)	4(+3) - 3(+3)		$1\nu_9 \ell = -1$	[84032]
	68394.941	(0.050)	4(+2) - 3(+2)		$1\nu_9 \ell = -1$	[84032]
	68405.342	(0.050)	4(+1) - 3(+1)		$1\nu_9 \ell = -1$	[84032]
	68406.824	(0.050)	4(+3) - 3(+3)		$1\nu_9 \ell = +1$	[84032]
	68407.856	(0.050)	4(0) - 3(0)		$1\nu_9 \ell = +1$	[84032]
	68409.668	(0.050)	4(+2) - 3(+2)		$1\nu_9 \ell = +1$	[84032]
	68446.336	(0.050)	4(+1) - 3(+1)		$1\nu_9 \ell = +1$	[84032]
	68447.100	(0.050)	4(+1) - 3(+1)		$2\nu_9 \ell = 0$	[86019]
	68448.633	(0.200)	4(0) - 3(0)		$2\nu_9 \ell = +2$	[86019]
	68448.875	(0.050)	4(0) - 3(0)		$2\nu_9 \ell = 0$	[86019]
	68491.993	(0.030)	4(+1) - 3(+1)		$1\nu_{10} \ell = +1$	[69063]
	68454.518	(0.200)	4(+1) - 3(+1)		$2\nu_9 \ell = +2$	[86019]
	68457.956	(0.200)	4(+2) - 3(+2)		$2\nu_9 \ell = +2$	[86019]
	68538.052	(0.030)	4(+3) - 3(+3)		$1\nu_{10} \ell = -1$	[69063]
	68547.148	(0.030)	4(+2) - 3(+2)		$1\nu_{10} \ell = -1$	[69063]
	68553.602	(0.030)	4(+1) - 3(+1)		$1\nu_{10} \ell = -1$	[69063]
	68554.251	(0.030)	4(+3) - 3(+3)		$1\nu_{10} \ell = +1$	[69063]
	68557.333	(0.030)	4(0) - 3(0)		$1\nu_{10} \ell = +1$	[69063]
	68558.447	(0.030)	4(+2) - 3(+2)		$1\nu_{10} \ell = +1$	[69063]
	68626.217	(0.030)	4(+1) - 3(+1)		$1\nu_{10} \ell = +1$	[69063]
	68737.665	(0.100)	4(+1) - 3(+1)		$2\nu_{10} \ell = -2$	[85015]
	68738.533	(0.100)	4(3) - 3(3)		$2\nu_{10} \ell = 0$	[85015]
	68740.904	(0.100)	4(2) - 3(2)		$2\nu_{10} \ell = 0$	[85015]
	68746.134	(0.100)	4(1) - 3(1)		$2\nu_{10} \ell = 0$	[85015]
	68747.724	(0.100)	4(0) - 3(0)		$2\nu_{10} \ell = 0$	[85015]
	68749.992	(0.100)	4(+2) - 3(+2)		$2\nu_{10} \ell = +2$	[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)		$1\nu_{10} \ell = +1$	[69063]
	85683.174	(0.060)	5(+2) - 4(+2)		$1\nu_{10} \ell = -1$	[69063]
	85684.002	(0.060)	5(+4) - 4(+4)		$1\nu_{10} \ell = +1$	[69063]
	85691.206	(0.060)	5(+1) - 4(+1)		$1\nu_{10} \ell = -1$	[69063]
	85692.374	(0.060)	5(+3) - 4(+3)		$1\nu_{10} \ell = +1$	[69063]
	85695.638	(0.060)	5(0) - 4(0)		$1\nu_{10} \ell = +1$	[69063]
	85697.750	(0.060)	5(+2) - 4(+2)		$1\nu_{10} \ell = +1$	[69063]
	85782.322	(0.060)	5(+1) - 4(+1)		$1\nu_{10} \ell = +1$	[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)		$1\nu_{10} \ell = +1$	[69063]
	102766.158	(0.090)	6(+5) - 5(+5)		$1\nu_{10} \ell = -1$	[69063]
	102787.743	(0.090)	6(+4) - 5(+4)		$1\nu_{10} \ell = -1$	[69063]
	102805.311	(0.090)	6(+3) - 5(+3)		$1\nu_{10} \ell = -1$	[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)	$J' K' - J'' K''$	$F' F'_1 - F'' F''_1$	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)	$J'(K_{-1}, K_{+1})$	$- J''(K_{-1}, K_{+1})$	ν_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)	$J'(K_{-1}, K_{+1})$	$- J''(K_{-1}, K_{+1})$	ν_1	Sym.	Ref.	
CH ₂ CH ¹³ CH ₃	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]	
	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]
asy-CH ₂ CHCH ₂ D		34966.94	(0.05)	2(1, 1)	- 1(1, 0)	0	A	[61013]
		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_t	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	CD ₂ CH ₂ CH ₂	CH ₂ CH ₂ CH ₂ ^a	CD ₂ CD ₂ 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]
	321844.590	(0.030)	11(10, 1) - 10(10, 0)	[87019]
D ₂ C-CH ₂ ∨ CH ₂	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)
$\text{CH}_3\ ^{13}\text{CH}_2\text{CH}_3$	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]			
$\text{CH}_3\text{CD}_2\text{CH}_3$	$\mu_b = 0.095(1)^a \text{ D}$		
$\text{CD}_3\text{CH}_2\text{CD}_3$	$\mu_b = 0.076(1)^a \text{ D}$		

^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	<i>A</i> ₁ <i>E</i>	[73048]
	24326.37	(0.05)	3(1, 2) - 3(0, 3)	1 1	<i>E</i> <i>A</i> ₂	[73048]
	24365.370	(0.030)	3(1, 2) - 3(0, 3)		<i>AE</i> + <i>EA</i>	[85023]
	24365.451	(0.030)	3(1, 2) - 3(0, 3)		<i>EE</i>	[85023]
	24365.531	(0.030)	3(1, 2) - 3(0, 3)		<i>AA</i>	[85023]
	25916.034	(0.030)	12(6, 7) - 13(5, 8)		<i>EE</i>	[85023]
	25916.258	(0.030)	12(6, 7) - 13(5, 8)		<i>AE</i>	[85023]
	25916.931	(0.030)	12(6, 7) - 13(5, 8)		<i>AA</i>	[85023]
	25917.154	(0.030)	12(6, 6) - 13(5, 9)		<i>EE</i>	[85023]
	25925.572	(0.030)	12(6, 7) - 13(5, 8)		<i>EE</i>	[85023]
	25925.804	(0.030)	12(6, 6) - 13(5, 9)		<i>AE</i>	[85023]
	25926.705	(0.030)	12(6, 6) - 13(5, 9)		<i>EE</i>	[85023]
	25926.452	(0.030)	12(6, 6) - 13(5, 9)		<i>AA</i>	[85023]
	26132.816	(0.030)	8(2, 6) - 7(3, 5)		<i>AA</i>	[85023]
	26133.035	(0.030)	8(2, 6) - 7(3, 5)		<i>EE</i>	[85023]
	26133.245	(0.030)	8(2, 6) - 7(3, 5)		<i>AE</i> + <i>EA</i>	[85023]
	26411.06	(0.05)	4(1, 3) - 4(0, 4)	1 2	<i>A</i> ₂ <i>A</i> ₁	[73048]
	26413.30	(0.05)	4(1, 3) - 4(0, 4)	1 2	<i>EE</i>	[73048]
	26415.55	(0.05)	4(1, 3) - 4(0, 4)	1 2	<i>A</i> ₂ <i>E</i>	[73048]
	26415.55	(0.05)	4(1, 3) - 4(0, 4)	1 2	<i>E</i> <i>A</i> ₁	[73048]
	26556.51	(0.05)	4(1, 3) - 4(0, 4)	1 1	<i>A</i> ₁ <i>A</i> ₂	[73048]
	26558.40	(0.05)	4(1, 3) - 4(0, 4)	1 1	<i>EE</i>	[73048]
	26560.30	(0.05)	4(1, 3) - 4(0, 4)	1 1	<i>A</i> ₁ <i>E</i>	[73048]
	26560.30	(0.05)	4(1, 3) - 4(0, 4)	1 1	<i>E</i> <i>A</i> 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	<i>A</i> ₂ <i>A</i> ₁	[67033]
	29337.18	(0.05)	5(1, 4) - 5(0, 5)	1 2	<i>EE</i>	[67033]
	29339.60	(0.05)	5(1, 4) - 5(0, 5)	1 2	<i>A</i> ₂ <i>E</i>	[67033]
	29339.60	(0.05)	5(1, 4) - 5(0, 5)	1 2	<i>E</i> <i>A</i> ₁	[67033]
	29525.87	(0.05)	5(1, 4) - 5(0, 5)	1 1	<i>A</i> ₁ <i>A</i> ₂	[67033]
	29527.91	(0.05)	5(1, 4) - 5(0, 5)	1 1	<i>EE</i>	[67033]
	29529.98	(0.05)	5(1, 4) - 5(0, 5)	1 1	<i>A</i> ₁ <i>E</i>	[67033]
	29529.98	(0.05)	5(1, 4) - 5(0, 5)	1 1	<i>E</i> <i>A</i> 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	<i>A</i> ₁ <i>A</i> ₂	[73084]
	36617.73	(0.05)	1(1, 1) - 0(0, 0)	1 1	<i>EE</i>	[73084]
	36619.24	(0.05)	1(1, 1) - 0(0, 0)	1 1	<i>A</i> ₁ <i>E</i>	[73084]
	36619.24	(0.05)	1(1, 1) - 0(0, 0)	1 1	<i>E</i> <i>A</i> ₂	[73084]
	36534.10	(0.05)	1(1, 1) - 0(0, 0)	1 2	<i>A</i> ₂ <i>A</i> ₁	[73084]
	36535.95	(0.05)	1(1, 1) - 0(0, 0)	1 2	<i>EE</i>	[73084]
	36537.80	(0.05)	1(1, 1) - 0(0, 0)	1 2	<i>A</i> ₂ <i>E</i>	[73084]
	36537.80	(0.05)	1(1, 1) - 0(0, 0)	1 2	<i>E</i> <i>A</i> 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	<i>A</i> ₂ <i>A</i> ₁	[73084]
	51427.45	(0.05)	2(1, 2) - 1(0, 1)	1 2	<i>EE</i>	[73084]
	51429.25	(0.05)	2(1, 2) - 1(0, 1)	1 2	<i>A</i> ₂ <i>E</i>	[73084]
	51429.25	(0.05)	2(1, 2) - 1(0, 1)	1 2	<i>E</i> <i>A</i> ₁	[73084]
	51514.95	(0.05)	2(1, 2) - 1(0, 1)	1 1	<i>A</i> ₁ <i>A</i> ₂	[73084]
	51516.55	(0.05)	2(1, 2) - 1(0, 1)	1 1	<i>EE</i>	[73084]
	51518.15	(0.05)	2(1, 2) - 1(0, 1)	1 1	<i>A</i> ₁ <i>E</i>	[73084]
	51518.15	(0.05)	2(1, 2) - 1(0, 1)	1 1	<i>E</i> <i>A</i> 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]

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]
<i>sym</i> -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	1ν ₈ - 1ν ₆	fe [81046]
	71896.242	(0.050)	3 - 3	1ν ₈ - 1ν ₆	fe [81046]
	71914.713	(0.050)	4 - 4	1ν ₈ - 1ν ₆	fe [81046]
	72195.871	(0.050)	18 - 17	1ν ₆₊₉ - 1ν ₈₊₉	Δ f [82036]
	72284.350	(0.050)	18 - 17	1ν ₆₊₉ - 1ν ₈₊₉	Δ e [82036]
	72524.001	(0.050)	3 - 2	1ν ₈₊₉ - 1ν ₆₊₉	Σ ⁺ [82036]
	76339.339	(0.050)	18 - 17	1ν ₆₊₉ - 1ν ₈₊₉	Σ ⁻ [82036]
	77317.949	(0.050)	15 - 14	1ν ₆₊₉ - 1ν ₈₊₉	Σ ⁺ [82036]
	77409.181	(0.050)	17 - 16	1ν ₆ - 1ν ₈	e [82036]
	77514.202	(0.050)	17 - 16	1ν ₆ - 1ν ₈	f [82036]
	77570.815	(0.050)	4 - 4	1ν ₈₊₉ - 1ν ₆₊₉	fe [82036]
	77572.418	(0.050)	3 - 3	1ν ₈₊₉ - 1ν ₆₊₉	ef [82036]
	77573.323	(0.050)	2 - 2	1ν ₈₊₉ - 1ν ₆₊₉	fe [82036]
	81008.656	(0.050)	19 - 18	1ν ₆₊₉ - 1ν ₈₊₉	Δ f [82036]
	81118.771	(0.050)	19 - 18	1ν ₆₊₉ - 1ν ₈₊₉	Δ e [82036]
	81324.066	(0.050)	3 - 2	1ν ₈₊₉ - 1ν ₆₊₉	Σ ⁺ [82036]
	82219.760	(0.050)	1 - 0	1ν ₈₊₉ - 1ν ₆₊₉	Σ ⁻ [82036]
	85148.237	(0.050)	19 - 18	1ν ₆₊₉ - 1ν ₈₊₉	Σ ⁻ [82036]
	86137.441	(0.050)	16 - 15	1ν ₆₊₉ - 1ν ₈₊₉	Σ ⁺ [82036]
	86190.631	(0.050)	18 - 17	1ν ₆ - 1ν ₈	e [82036]
	86303.186	(0.050)	18 - 17	1ν ₆ - 1ν ₈	f [82036]
	89428.244	(0.050)	2 - 1	1ν ₈ - 1ν ₆	e [82036]
	89437.861	(0.050)	2 - 1	1ν ₈ - 1ν ₆	f [82036]
	89821.699	(0.050)	10 - 19	1ν ₆₊₉ - 1ν ₈₊₉	Δ f [82036]
	89956.981	(0.050)	10 - 19	1ν ₆₊₉ - 1ν ₈₊₉	Δ e [82036]
	90122.305	(0.050)	5 - 4	1ν ₈₊₉ - 1ν ₆₊₉	Σ ⁺ [82036]
	91026.942	(0.050)	2 - 1	1ν ₈₊₉ - 1ν ₆₊₉	Σ ⁻ [82036]
	93956.940	(0.050)	20 - 19	1ν ₆₊₉ - 1ν ₈₊₉	Σ ⁻ [82036]
	94955.928	(0.050)	17 - 16	1ν ₆₊₉ - 1ν ₈₊₉	Σ ⁺ [82036]
	94972.022	(0.050)	19 - 18	1ν ₆ - 1ν ₈	e [82036]
	95092.267	(0.050)	19 - 18	1ν ₆ - 1ν ₈	f [82036]
	98635.136	(0.050)	21 - 20	1ν ₆₊₉ - 1ν ₈₊₉	Δ f [82036]
	98799.479	(0.050)	21 - 20	1ν ₆₊₉ - 1ν ₈₊₉	Δ e [82036]
	102765.404	(0.050)	21 - 20	1ν ₆₊₉ - 1ν ₈₊₉	Σ ⁻ [82036]
	103753.379	(0.050)	20 - 19	1ν ₆ - 1ν ₈	e [82036]
	103773.020	(0.050)	18 - 17	1ν ₆₊₉ - 1ν ₈₊₉	Σ ⁺ [82036]
	103881.484	(0.050)	20 - 19	1ν ₆ - 1ν ₈	f [82036]
	103995.578	(0.050)	3 - 2	1ν ₈₊₉ - 1ν ₆₊₉	e [82036]
	106987.262	(0.050)	4 - 3	1ν ₈ - 1ν ₆	e [82036]
	107005.664	(0.050)	4 - 3	1ν ₈ - 1ν ₆	f [82036]
	107448.891	(0.050)	22 - 21	1ν ₆₊₉ - 1ν ₈₊₉	f [82036]
	107646.637	(0.050)	22 - 21	1ν ₆₊₉ - 1ν ₈₊₉	Δ e [82036]
	107713.512	(0.050)	7 - 6	1ν ₈₊₉ - 1ν ₆₊₉	Σ ⁺ [82036]
	108640.399	(0.050)	4 - 3	1ν ₈₊₉ - 1ν ₆₊₉	Σ ⁻ [82036]
	111573.608	(0.050)	22 - 21	1ν ₆₊₉ - 1ν ₈₊₉	Σ ⁻ [82036]
	112534.685	(0.050)	21 - 20	1ν ₆ - 1ν ₈	e [82036]
	112588.369	(0.050)	19 - 18	1ν ₆₊₉ - 1ν ₈₊₉	Σ ⁺ [82036]
	112670.794	(0.050)	21 - 20	1ν ₆ - 1ν ₈	f [82036]
	112802.051	(0.050)	4 - 3	1ν ₈₊₉ - 1ν ₆₊₉	f [82036]
	115766.433	(0.050)	5 - 4	1ν ₈ - 1ν ₆	e [82036]
	115789.016	(0.050)	5 - 4	1ν ₈ - 1ν ₆	f [82036]
	116263.138	(0.050)	23 - 22	1ν ₆₊₉ - 1ν ₈₊₉	Δ f [82036]
	116498.772	(0.050)	23 - 22	1ν ₆₊₉ - 1ν ₈₊₉	Δ e [82036]
	116506.680	(0.050)	8 - 7	1ν ₈₊₉ - 1ν ₆₊₉	Σ ⁺ [82036]
	117446.561	(0.050)	5 - 4	1ν ₈₊₉ - 1ν ₆₊₉	Σ ⁻ [82036]
	120381.531	(0.050)	23 - 22	1ν ₆₊₉ - 1ν ₈₊₉	Σ ⁻ [82036]
	121315.959	(0.050)	22 - 21	1ν ₆ - 1ν ₈	e [82036]
	121401.629	(0.050)	20 - 19	1ν ₆₊₉ - 1ν ₈₊₉	Σ ⁺ [82036]
	121460.178	(0.050)	22 - 21	1ν ₆ - 1ν ₈	f [82036]
	121608.007	(0.050)	5 - 4	1ν ₈₊₉ - 1ν ₆₊₉	Δ e [82036]
	124545.399	(0.050)	6 - 5	1ν ₈ - 1ν ₆	e [82036]
	124572.043	(0.050)	6 - 5	1ν ₈ - 1ν ₆	f [82036]
	125077.626	(0.050)	24 - 23	1ν ₆₊₉ - 1ν ₈₊₉	Δ f [82036]
	125298.468	(0.050)	9 - 8	1ν ₈₊₉ - 1ν ₆₊₉	Σ ⁺ [82036]
	125356.186	(0.050)	24 - 23	1ν ₆₊₉ - 1ν ₈₊₉	Δ e [82036]
	126252.506	(0.050)	6 - 5	1ν ₈₊₉ - 1ν ₆₊₉	Σ ⁻ [82036]
	129189.080	(0.050)	24 - 23	1ν ₆₊₉ - 1ν 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	$1\nu_6 - 1\nu_8$	<i>e</i> [82036]
	130212.435	(0.050)	21 - 20	$1\nu_{6+9} - 1\nu_{8+9}$	Σ^+ [82036]
	130249.652	(0.050)	23 - 22	$1\nu_6 - 1\nu_8$	<i>f</i> [82036]
	130414.035	(0.050)	6 - 5	$1\nu_{8+9} - 1\nu_{6+9}$	Δf [82036]
	133324.095	(0.050)	7 - 6	$1\nu_8 - 1\nu_6$	<i>e</i> [82036]
	133354.629	(0.050)	7 - 6	$1\nu_8 - 1\nu_6$	<i>f</i> [82036]
	133892.550	(0.050)	25 - 24	$1\nu_{8+9} - 1\nu_{6+9}$	Δf [82036]
	134088.978	(0.050)	10 - 9	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [82036]
	134219.116	(0.050)	25 - 24	$1\nu_{6+9} - 1\nu_{8+9}$	Δe [82036]
	135058.018	(0.050)	7 - 6	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [82036]
	139218.165	(0.050)	7 - 6	$1\nu_{8+9} - 1\nu_{6+9}$	Δe [82036]
	139219.435	(0.050)	7 - 6	$1\nu_{8+9} - 1\nu_{6+9}$	Δf [82036]
	142102.507	(0.050)	8 - 7	$1\nu_8 - 1\nu_6$	<i>e</i> [82036]
	142136.842	(0.050)	8 - 7	$1\nu_8 - 1\nu_6$	<i>f</i> [82036]
	142707.939	(0.050)	26 - 25	$1\nu_{8+9} - 1\nu_{6+9}$	Δf [82036]
	142878.315	(0.050)	11 - 10	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [82036]
	143088.041	(0.050)	26 - 25	$1\nu_{6+9} - 1\nu_{8+9}$	Δe [82036]
	143863.183	(0.050)	8 - 7	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [82036]
	148022.182	(0.050)	8 - 7	$1\nu_{8+9} - 1\nu_{6+9}$	Δe [82036]
	148024.537	(0.050)	8 - 7	$1\nu_{8+9} - 1\nu_{6+9}$	Δf [82036]
	150880.704	(0.050)	9 - 8	$1\nu_8 - 1\nu_6$	<i>e</i> [82036]
	150918.629	(0.050)	9 - 8	$1\nu_8 - 1\nu_6$	<i>f</i> [82036]
	151666.863	(0.050)	12 - 11	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [82036]
	152667.962	(0.050)	9 - 8	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [82036]
	156825.143	(0.050)	9 - 8	$1\nu_{8+9} - 1\nu_{6+9}$	Δe [82036]
	156829.215	(0.050)	9 - 8	$1\nu_{8+9} - 1\nu_{6+9}$	Δf [82036]
	159658.615	(0.050)	10 - 9	$1\nu_8 - 1\nu_6$	<i>e</i> [82036]
	160454.614	(0.050)	13 - 12	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^+ [82036]
	161472.445	(0.050)	10 - 9	$1\nu_{8+9} - 1\nu_{6+9}$	Σ^- [82036]
	165627.043	(0.050)	10 - 9	$1\nu_{8+9} - 1\nu_{6+9}$	Δe [82036]
	165633.481	(0.050)	10 - 9	$1\nu_{8+9} - 1\nu_{6+9}$	Δf [82036]
	168436.178	(0.050)	11 - 10	$1\nu_8 - 1\nu_6$	<i>e</i> [82036]
	168480.873	(0.050)	11 - 10	$1\nu_8 - 1\nu_6$	<i>f</i> [82036]
	174427.490	(0.050)	11 - 10	$1\nu_{8+9} - 1\nu_{6+9}$	Δe [82036]
	174437.376	(0.050)	11 - 10	$1\nu_{8+9} - 1\nu_{6+9}$	Δf [82036]
HCCCD	40851.35	(0.05)	5 - 4	$1\nu_6$	<i>e</i> [81047]
	40872.61	(0.05)	5 - 4	$1\nu_6$	<i>f</i> [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	$1\nu_6$	<i>e</i> [81047]
	49047.01	(0.05)	6 - 5	$1\nu_6$	<i>f</i> [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	$1\nu_6$	<i>e</i> [81047]
	57221.41	(0.05)	7 - 6	$1\nu_6$	<i>f</i> [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	$1\nu_6$	<i>e</i> [81047]
	65395.71	(0.05)	8 - 7	$1\nu_6$	<i>f</i> [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	$1\nu_6$	<i>e</i> [81047]
	73569.92	(0.05)	9 - 8	$1\nu_6$	<i>f</i> [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 ν_7 , 1 ν_8	[81047]
	73758.59	(0.05)	9 - 8	1 ν_6 , 1 ν_9	[81047]
	73780.22	(0.05)	9 - 8	2 ν_6 , 1 ν_9	[81047]
	32344.532	(0.050)	6 - 7	1 ν_{6+9} - 1 ν_{8+9} Δ f	[84037]
	33077.941	(0.050)	6 - 7	1 ν_6 - 1 ν_8 f	[84037]
	33109.382	(0.050)	6 - 7	1 ν_6 - 1 ν_8 e	[84037]
	33516.980	(0.050)	19 - 18	1 ν_{8+9} - 1 ν_{6+9} Σ^+	[84037]
	35016.295	(0.050)	9 - 10	1 ν_{6+9} - 1 ν_{8+9} Σ^+	[84037]
	35227.837	(0.050)	16 - 15	1 ν_8 - 1 ν_6 e	[84037]
	35298.118	(0.050)	16 - 15	1 ν_8 - 1 ν_6 f	[84037]
	36167.930	(0.050)	16 - 15	1 ν_{8+9} - 1 ν_{6+9} Δ e	[84037]
	36204.173	(0.050)	16 - 15	1 ν_{8+9} - 1 ν_{6+9} Δ f	[84037]
	37984.890	(0.050)	16 - 15	1 ν_{8+9} - 1 ν_{6+9} Σ^-	[84037]
	38179.389	(0.050)	5 - 6	1 ν_{6+9} - 1 ν_{8+9} Σ^-	[84037]
	39974.857	(0.050)	5 - 6	1 ν_{6+9} - 1 ν_{8+9} Δ e	[84037]
	40689.422	(0.050)	5 - 6	1 ν_6 - 1 ν_8 f	[84037]
	40716.456	(0.050)	5 - 6	1 ν_6 - 1 ν_8 e	[84037]
	41127.064	(0.050)	10 - 19	1 ν_{8+9} - 1 ν_{6+9} Σ^+	[84037]
	42639.419	(0.050)	8 - 9	1 ν_{6+9} - 1 ν_{8+9} Σ^+	[84037]
	42806.715	(0.050)	17 - 16	1 ν_8 - 1 ν_6 e	[84037]
	42881.229	(0.050)	17 - 16	1 ν_8 - 1 ν_6 f	[84037]
	43760.288	(0.050)	17 - 16	1 ν_{8+9} - 1 ν_{6+9} Δ e	[84037]
	43807.142	(0.050)	17 - 16	1 ν_{8+9} - 1 ν_{6+9} Δ f	[84037]
	45811.595	(0.050)	4 - 5	1 ν_{6+9} - 1 ν_{8+9} Σ^-	[84037]
	45585.334	(0.050)	17 - 16	1 ν_{8+9} - 1 ν_{6+9} Σ^-	[84037]
	47607.257	(0.050)	4 - 5	1 ν_{6+9} - 1 ν_{8+9} Δ f	[84037]
	48303.674	(0.050)	4 - 5	1 ν_6 - 1 ν_8 f	[84037]
	48326.218	(0.050)	4 - 5	1 ν_6 - 1 ν_8 e	[84037]
	48737.095	(0.050)	21 - 20	1 ν_{8+9} - 1 ν_{6+9} Σ^+	[84037]
	50264.776	(0.050)	7 - 8	1 ν_{6+9} - 1 ν_{8+9} Σ^+	[84037]
	50382.694	(0.050)	18 - 17	1 ν_8 - 1 ν_6 e	[84037]
	50461.391	(0.050)	18 - 17	1 ν_8 - 1 ν_6 f	[84037]
	51347.882	(0.050)	18 - 17	1 ν_{8+9} - 1 ν_{6+9} Δ e	[84037]
	51407.438	(0.050)	18 - 17	1 ν_{8+9} - 1 ν_{6+9} Δ f	[84037]
	53182.728	(0.050)	18 - 17	1 ν_{8+9} - 1 ν_{6+9} Σ^-	[84037]
	53446.647	(0.050)	3 - 4	1 ν_{6+9} - 1 ν_{8+9} Σ^-	[84037]
	55242.595	(0.050)	3 - 4	1 ν_{6+9} - 1 ν_{8+9} Δ e	[84037]
	55920.701	(0.050)	3 - 4	1 ν_6 - 1 ν_8 f	[84037]
	55938.802	(0.050)	3 - 4	1 ν_6 - 1 ν_8 e	[84037]
	56347.221	(0.050)	22 - 21	1 ν_{8+9} - 1 ν_{6+9} Σ^+	[84037]
	57892.468	(0.050)	6 - 7	1 ν_{6+9} - 1 ν_{8+9} Σ^+	[84037]
	57955.823	(0.050)	19 - 18	1 ν_8 - 1 ν_6 e	[84037]
	58038.667	(0.050)	19 - 18	1 ν_8 - 1 ν_6 f	[84037]
	58930.412	(0.050)	19 - 18	1 ν_{8+9} - 1 ν_{6+9} Δ e	[84037]
	59004.969	(0.050)	19 - 18	1 ν_{8+9} - 1 ν_{6+9} Δ f	[84037]
	60777.046	(0.050)	19 - 18	1 ν_{8+9} - 1 ν_{6+9} Σ^-	[84037]
	61084.375	(0.050)	2 - 3	1 ν_{6+9} - 1 ν_{8+9} Σ^-	[84037]
	62880.639	(0.050)	2 - 3	1 ν_{6+9} - 1 ν_{8+9} Δ f	[84037]
	63540.539	(0.050)	2 - 3	1 ν_6 - 1 ν_8 f	[84037]
	63554.142	(0.050)	2 - 3	1 ν_6 - 1 ν_8 e	[84037]
63957.678	(0.050)	23 - 22	1 ν_{8+9} - 1 ν_{6+9} Σ^+	[84037]	
65522.258	(0.050)	5 - 6	1 ν_{6+9} - 1 ν_{8+9} Σ^+	[84037]	
65526.057	(0.050)	20 - 19	1 ν_8 - 1 ν_6 e	[84037]	
65613.063	(0.050)	20 - 19	1 ν_8 - 1 ν_6 f	[84037]	
66507.655	(0.050)	20 - 19	1 ν_{8+9} - 1 ν_{6+9} Δ e	[84037]	
66599.864	(0.050)	20 - 19	1 ν_{8+9} - 1 ν_{6+9} Δ f	[84037]	
68368.383	(0.050)	20 - 19	1 ν_{8+9} - 1 ν_{6+9} Σ^-	[84037]	
68725.135	(0.050)	1 - 2	1 ν_{6+9} - 1 ν_{8+9} Σ^-	[84037]	
71163.138	(0.050)	1 - 2	1 ν_6 - 1 ν_8 f	[84037]	
71172.216	(0.050)	1 - 2	1 ν_6 - 1 ν_8 e	[84037]	
71568.712	(0.050)	24 - 23	1 ν_{8+9} - 1 ν_{6+9} Σ^+	[84037]	
73093.418	(0.050)	21 - 20	1 ν_8 - 1 ν_6 e	[84037]	
73155.331	(0.050)	4 - 5	1 ν_{6+9} - 1 ν_{8+9} Σ^+	[84037]	
73184.521	(0.050)	21 - 20	1 ν_8 - 1 ν_6 f	[84037]	
74079.297	(0.050)	21 - 20	1 ν_{8+9} - 1 ν_{6+9} Δ e	[84037]	
74191.989	(0.050)	21 - 20	1 ν_{8+9} - 1 ν_{6+9} Δ f	[84037]	
75956.650	(0.050)	21 - 20	1 ν_{8+9} - 1 ν_{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

C₄H₄

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

C₄H₄

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)	1ν ₁₃	[80032]
	33179.8	(0.3)	4(1, 4) - 3(1, 3)	2ν ₁₃	[70061]
	33251.7	(0.3)	4(1, 4) - 3(1, 3)	3ν 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)	1ν ₁₈	[80032]
	33789.618	(0.050)	4(2, 2) - 3(2, 1)		[80032]
	33807.800	(0.050)	4(2, 3) - 3(2, 2)	1ν ₁₈	[80032]
	33817.130	(0.050)	4(3, 2) - 3(3, 1)	1ν ₁₈	[80032]
	33817.130	(0.050)	4(3, 1) - 3(3, 0)	1ν ₁₈	[80032]
	33828.670	(0.050)	4(2, 2) - 3(2, 1)	1ν ₁₈	[80032]
	33837.553	(0.050)	4(0, 4) - 3(0, 3)	1ν ₁₃	[80032]
	33861.830	(0.050)	4(2, 3) - 3(2, 2)	1ν ₁₃	[80032]
	33871.151	(0.050)	4(3, 2) - 3(3, 1)	1ν ₁₃	[80032]
	33871.151	(0.050)	4(3, 1) - 3(3, 0)	1ν ₁₃	[80032]
	33885.830	(0.050)	4(2, 2) - 3(2, 1)	1ν ₁₃	[80032]
	33955.0	(0.5)	4(2, 3) - 3(2, 2)	2ν ₁₃	[70061]
	33964.0	(0.5)	4(3, 2) - 3(3, 1)	2ν ₁₃	[70061]
	33964.0	(0.5)	4(3, 1) - 3(3, 0)	2ν ₁₃	[70061]
	33980.3	(0.5)	4(2, 2) - 3(2, 1)	2ν ₁₃	[70061]
	34495.050	(0.050)	4(1, 3) - 3(1, 2)		[80032]
	34524.050	(0.050)	4(1, 3) - 3(1, 2)	1ν ₁₈	[80032]
	34554.0	(0.3)	4(1, 3) - 3(1, 2)	2ν ₁₈	[70061]
	34608.790	(0.050)	4(1, 3) - 3(1, 2)	1ν ₁₃	[80032]
	34720.0	(0.3)	4(1, 3) - 3(1, 2)	2ν ₁₃	[70061]
	34831.0	(0.3)	4(1, 3) - 3(1, 2)	3ν ₁₃	[70061]

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

Parameter	$\overline{\text{HC=CHC=CH}_2}$	$\text{H}^{13}\text{C}=\overline{\text{CHC=CH}_2}$	$\overline{\text{HC=CHC=}}^{13}\text{CH}_2$
<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.
CHCHCCH ₂	27207.47	(0.10)	2(1, 1) - 1(1, 0)	[86013]
	29454.45	(0.10)	6(1, 5) - 6(1, 6)	[86013]
CH ₂	34760.46	(0.10)	11(2, 9) - 11(2, 10)	[86013]
	35015.64	(0.10)	16(3, 13) - 16(3, 14)	[86013]
C	36540.88	(0.10)	3(1, 3) - 2(1, 2)	[86013]
/ \	38436.00	(0.10)	3(0, 3) - 2(0, 2)	[86013]
HC=CH	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]
	38391.30	(0.10)	3(2, 1) - 2(2, 0)	[86013]
CHCHC ¹³ CH ₂	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)	$J'K'm_H^e - J''K''m_H^e$	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)	$J'K'm_H^{\prime} - J''K''m_H''$	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 (C₄H₆) 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)x10 ⁻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)x10 ⁻⁵		
$\theta(a,i)$	47.55(19) ^o	48.454(13) ^o	
I _{α} (u Å 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 $v_{24}=1$ 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 ($u \text{ \AA}^2$)	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)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_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 ₅ (1 ₀) 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}			
$2\chi_{\text{aa}} - \chi_{\text{bb}} - \chi_{\text{cc}}$	$-5.9(3) \times 10^{-6} \text{erg/G}^2 \cdot \text{mol}$			
$-\chi_{\text{aa}} + 2\chi_{\text{bb}} - \chi_{\text{cc}}$	$21.1(3) \times 10^{-6} \text{erg/G}^2 \cdot \text{mol}$			

^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)	$J'(K_-, K_+) - J''(K_-, K_+)$	Ref.
$\text{CHCHCH}_2\text{CH}_2$ 	8978.350	(0.050)	7(6, 1) - 7(6, 2)	[65029]
	10799.790	(0.050)	6(5, 1) - 6(5, 2)	[65029]
	12117.960	(0.050)	12(10, 2) - 12(10, 3)	[65029]
	12505.920	(0.050)	5(4, 1) - 5(4, 2)	[65029]
	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]	
$^{13}\text{CHCHCH}_2\text{CH}_2$ 	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]
CHCH ¹³ CH ₂ CH ₂	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]

TABLE 23.3. Microwave spectrum of cyclobutene — Continued

C₄H₆

Isotopic species	Frequeny (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)
V_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_i	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 cyclopropane — Continued

C₄H₆

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_i	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)	18998.1(1)
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]
	24503.060	(0.050)	2(0, 2) - 1(0, 1)	[70062]
CH ₂ C ¹³ CH ₂ CH ₂ ¹³ C ₃	26047.220	(0.050)	2(1, 1) - 1(1, 0)	[70062]
	12156.350	(0.050)	1(0, 1) - 0(0, 0)	[70062]
	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 [present]</u>		
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 [68043]</u>		
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 ₈	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.
<i>c</i> -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	<i>E</i>		[68043]
	27093.92	(0.10)	7(2, 5) - 7(1, 6)	2	<i>A</i>		[68043]
	27220.76	(0.10)	7(2, 5) - 7(1, 6)				[68043]
	27464.68	(0.10)	3(1, 3) - 2(1, 2)	2	<i>A</i>		[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	<i>E</i>		[68043]
	28272.40	(0.10)	6(1, 5) - 6(0, 6)	2	<i>A</i>		[68043]
	28763.56	(0.10)	6(1, 5) - 6(0, 6)				[68043]
	28954.80	(0.10)	3(0, 3) - 2(0, 2)	2	<i>E</i>		[68043]
	28955.50	(0.10)	3(0, 3) - 2(0, 2)	2	<i>A</i>		[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	<i>E</i>		[68043]
	29535.12	(0.10)	8(2, 6) - 8(1, 7)	2	<i>A</i>		[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	<i>E</i>		[68043]
	31184.88	(0.10)	3(1, 2) - 2(1, 1)	2	<i>A</i>		[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	<i>E</i>		[68043]
	33448.66	(0.10)	9(2, 7) - 9(1, 8)	2	<i>A</i>		[68043]
33958.86	(0.10)	9(2, 7) - 9(1, 8)				[68043]	
34975.72	(0.10)	3(2, 2) - 3(1, 3)				[68043]	
<i>c</i> - 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)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1}) \nu_1$	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)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	v_1	Sym.	Vib. state	Ref.
	17065.04	(0.10)	7(1, 7) - 7(0, 7)	0	<i>A</i>	2ν ₁	[68043]
	17074.78	(0.10)	7(1, 7) - 7(0, 7)	0	<i>E</i>	2ν ₁	[68043]
	17091.24	(0.10)	7(1, 7) - 7(0, 7)	0	<i>A</i>	1ν ₁	[68043]
	17091.54	(0.10)	7(1, 7) - 7(0, 7)	0	<i>E</i>	1ν 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	<i>A</i>	2ν ₁	[68043]
	17403.40	(0.10)	6(1, 6) - 6(0, 6)	0	<i>E</i>	2ν ₁	[68043]
	17418.20	(0.10)	6(1, 6) - 6(0, 6)	0	<i>A</i>	1ν ₁	[68043]
	17418.60	(0.10)	6(1, 6) - 6(0, 6)	0	<i>E</i>	1ν 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	<i>A</i>	2ν ₁	[68043]
	17688.86	(0.10)	5(1, 5) - 5(0, 5)	0	<i>E</i>	2ν ₁	[68043]
	17702.40	(0.10)	5(1, 5) - 5(0, 5)	0	<i>A</i>	1ν ₁	[68043]
	17702.70	(0.10)	5(1, 5) - 5(0, 5)	0	<i>E</i>	1ν 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	<i>A</i>	2ν ₁	[68043]
	17928.80	(0.10)	4(1, 4) - 4(0, 4)	0	<i>E</i>	2ν 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	<i>A,E</i>	2ν 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	<i>A</i>	2ν ₁	[68043]
	18713.66	(0.10)	3(1, 2) - 3(0, 3)	0	<i>E</i>	2ν ₁	[68043]
	18725.60	(0.10)	3(1, 2) - 3(0, 3)	0	<i>A,E</i>	1ν 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	<i>A</i>		[68043]
	18766.22	(0.10)	3(1, 2) - 3(0, 3)	1	<i>E</i>		[68043]
	18914.20	(0.10)	4(1, 3) - 4(0, 4)	0	<i>A</i>	2ν ₁	[68043]
	18915.30	(0.10)	4(1, 3) - 4(0, 4)	0	<i>E</i>	2ν ₁	[68043]
	18926.10	(0.10)	4(1, 3) - 4(0, 4)	0	<i>A,E</i>	1ν 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	<i>A</i>		[68043]
	18966.26	(0.10)	4(1, 3) - 4(0, 4)	1	<i>E</i>		[68043]
	19168.80	(0.10)	5(1, 4) - 5(0, 5)	0	<i>A</i>	2ν ₁	[68043]
	19169.92	(0.10)	5(1, 4) - 5(0, 5)	0	<i>E</i>	2ν ₁	[68043]
	19179.42	(0.10)	5(1, 4) - 5(0, 5)	0	<i>A,E</i>	1ν 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	<i>A</i>		[68043]
	19218.86	(0.10)	5(1, 4) - 5(0, 5)	1	<i>E</i>		[68043]
	19477.53	(0.10)	6(1, 5) - 6(0, 6)	0	<i>A</i>	2ν ₁	[68043]
	19478.67	(0.10)	6(1, 5) - 6(0, 6)	0	<i>E</i>	2ν ₁	[68043]
	19486.46	(0.10)	6(1, 5) - 6(0, 6)	0	<i>A,E</i>	1ν ₁	[68043]
	19523.06	(0.10)	6(1, 5) - 6(0, 6)	1	<i>A</i>		[68043]
	19524.62	(0.10)	6(1, 5) - 6(0, 6)	1	<i>E</i>		[68043]
	19526.14	(0.10)	6(1, 5) - 6(0, 6)	0			[68043]
	19842.45	(0.10)	7(1, 6) - 7(0, 7)	0	<i>A</i>	2ν ₁	[68043]
	19843.61	(0.10)	7(1, 6) - 7(0, 7)	0	<i>E</i>	2ν ₁	[68043]
	19849.20	(0.10)	7(1, 6) - 7(0, 7)	0	<i>A,E</i>	1ν ₁	[68043]
	19884.73	(0.10)	7(1, 6) - 7(0, 7)	1	<i>A</i>		[68043]
	19886.41	(0.10)	7(1, 6) - 7(0, 7)	1	<i>E</i>		[68043]
	19894.69	(0.10)	7(1, 6) - 7(0, 7)	0			[68043]
	20265.59	(0.10)	8(1, 7) - 8(0, 8)	0	<i>A</i>	2ν ₁	[68043]
	20266.70	(0.10)	8(1, 7) - 8(0, 8)	0	<i>E</i>	2ν ₁	[68043]
	20269.88	(0.10)	8(1, 7) - 8(0, 8)	0	<i>A,E</i>	1ν ₁	[68043]
	20304.14	(0.10)	8(1, 7) - 8(0, 8)	1	<i>A</i>		[68043]
	20305.92	(0.10)	8(1, 7) - 8(0, 8)	1	<i>E</i>		[68043]
	20322.18	(0.10)	8(1, 7) - 8(0, 8)	0			[68043]
	20749.27	(0.10)	9(1, 8) - 9(0, 9)	0	<i>A</i>	2ν ₁	[68043]
	20750.38	(0.10)	9(1, 8) - 9(0, 9)	0	<i>E</i>	2ν ₁	[68043]
	20750.84	(0.10)	9(1, 8) - 9(0, 9)	0	<i>A,E</i>	1ν ₁	[68043]
	20783.64	(0.10)	9(1, 8) - 9(0, 9)	1	<i>A</i>		[68043]
	20785.47	(0.10)	9(1, 8) - 9(0, 9)	1	<i>E</i>		[68043]
	20811.02	(0.10)	9(1, 8) - 9(0, 9)	0			[68043]
	21294.66	(0.10)	10(1, 9) - 10(0, 10)	0	<i>A,E</i>	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.
	21296.28	(0.10)	10(1, 9) - 10(0,10)	0	<i>A</i>	2ν ₁	[68043]
	21297.42	(0.10)	10(1, 9) - 10(0,10)	0	<i>E</i>	2ν ₁	[68043]
	21325.93	(0.10)	10(1, 9) - 10(0,10)	1	<i>A</i>		[68043]
	21327.87	(0.10)	10(1, 9) - 10(0,10)	1	<i>E</i>		[68043]
	21363.88	(0.10)	10(1, 9) - 10(0,10)				[68043]
	21904.18	(0.10)	11(1,10) - 11(0,11)	0	<i>A,E</i>	1ν ₁	[68043]
	21909.25	(0.10)	11(1,10) - 11(0,11)	0	<i>A</i>	2ν ₁	[68043]
	21910.41	(0.10)	11(1,10) - 11(0,11)	0	<i>E</i>	2ν ₁	[68043]
	21933.64	(0.10)	11(1,10) - 11(0,11)	1	<i>A</i>		[68043]
	21935.76	(0.10)	11(1,10) - 11(0,11)	1	<i>E</i>		[68043]
	21983.88	(0.10)	11(1,10) - 11(0,11)				[68043]
	22582.60	(0.10)	12(1,11) - 12(0,12)	0	<i>A,E</i>	1ν ₁	[68043]
	22591.36	(0.10)	12(1,11) - 12(0,12)	0	<i>A</i>	2ν ₁	[68043]
	22592.61	(0.10)	12(1,11) - 12(0,12)	0	<i>E</i>	2ν ₁	[68043]
	22610.08	(0.10)	12(1,11) - 12(0,12)	1	<i>A</i>		[68043]
	22612.34	(0.10)	12(1,11) - 12(0,12)	1	<i>E</i>		[68043]
	22674.14	(0.10)	12(1,11) - 12(0,12)				[68043]
	23334.00	(0.10)	13(1,12) - 13(0,13)	0	<i>A,E</i>	1ν ₁	[68043]
	23346.40	(0.10)	13(1,12) - 13(0,13)	0	<i>A</i>	2ν ₁	[68043]
	23347.60	(0.10)	13(1,12) - 13(0,13)	0	<i>E</i>	2ν ₁	[68043]
	23438.14	(0.10)	13(1,12) - 13(0,13)				[68043]
	24160.00	(0.10)	14(1,13) - 14(0,14)	0	<i>A,E</i>	1ν ₁	[68043]
	24177.20	(0.10)	14(1,13) - 14(0,14)	0	<i>A</i>	2ν ₁	[68043]
	24178.40	(0.10)	14(1,13) - 14(0,14)	0	<i>E</i>	2ν ₁	[68043]
	24279.38	(0.10)	14(1,13) - 14(0,14)				[68043]
	24461.32	(0.10)	3(1, 3) - 2(1, 2)	1	<i>A</i>		[68043]
	24461.46	(0.10)	3(1, 3) - 2(1, 2)	1	<i>E</i>		[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	<i>A</i>		[68043]
	24755.88	(0.10)	3(1, 2) - 2(1, 1)	1	<i>E</i>		[68043]
	24787.28	(0.10)	3(1, 2) - 2(1, 1)				[68043]
	25065.28	(0.10)	15(1,14) - 15(0,15)	0	<i>A,E</i>	1ν ₁	[68043]
	25087.42	(0.10)	15(1,14) - 15(0,15)	0	<i>A</i>	2ν ₁	[68043]
	25088.60	(0.10)	15(1,14) - 15(0,15)	0	<i>E</i>	2ν 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]
	39996.34	(0.10)	5(2, 3) - 4(2, 2)				[79033]
s-CH ₂ CHCH ₂ ¹³ CH ₃	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_t	Sym.	Vib. state	Ref.
s-CD ₂ CD 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	$\text{CD}_3\text{CD}_2\text{CD}_3$	$\text{CD}_3\text{CHCHCD}_3$
<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</u> ^a [75058]			
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</u> [75058]			
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 (cm ⁻¹)			-74.(11)
Δ ₀ (MHz)	-9.659(58)		
ρ	0.05620(20)		
β (rad)	0.5172(12)		
<u>Electric Dipole Moment</u> [61014]			
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)		<i>AE + EA</i>		[61014]
	23524.94	(0.10)	7(7, 1) - 7(6, 2)		<i>EE</i>		[61014]
	23525.58	(0.10)	7(7, 1) - 7(6, 2)		<i>AA</i>		[61014]
	23993.911	(0.030)	8(8, 0) - 8(7, 1)		<i>AE</i>		[75058]
	23994.287	(0.030)	8(8, 0) - 8(7, 1)		<i>EA</i>		[75058]
	23994.821	(0.030)	8(8, 0) - 8(7, 1)		<i>EE</i>		[75058]
	23995.551	(0.030)	8(8, 0) - 8(7, 1)		<i>AA</i>		[75058]
	24638.80	(0.10)	9(6, 3) - 9(5, 4)				[61014]
	26574.382	(0.030)	8(8, 1) - 8(7, 2)		<i>EA</i>		[75058]
	26574.774	(0.030)	8(8, 1) - 8(7, 2)		<i>AE</i>		[75058]
	26575.365	(0.030)	8(8, 1) - 8(7, 2)		<i>EE</i>		[75058]
	26576.146	(0.030)	8(8, 1) - 8(7, 2)		<i>AA</i>		[75058]
	28121.48	(0.10)	6(3, 3) - 6(2, 4)				[61014]
	28219.237	(0.030)	9(9, 0) - 9(8, 1)		<i>AE</i>		[75058]
	28220.382	(0.030)	9(9, 0) - 9(8, 1)		<i>EE</i>		[75058]
	28221.066	(0.030)	9(9, 0) - 9(8, 1)		<i>AA</i>		[75058]
	28330.145	(0.030)	9(9, 0) - 9(8, 1)		<i>EA</i>		[75058]
	28557.285	(0.10)	5(2, 3) - 5(1, 4)				[61014]
	28759.698	(0.10)	4(2, 3) - 4(1, 4)		<i>A₂A₁</i>	<i>1ν₂</i>	[75058]
	28765.930	(0.10)	4(2, 3) - 4(1, 4)		<i>EE</i>	<i>1ν₂</i>	[75058]
	28771.06	(0.10)	4(1, 3) - 4(0, 4)				[61014]
	28772.171	(0.10)	4(1, 3) - 4(0, 4)	<i>A₂</i>	<i>E + EA₁</i>	<i>1ν₂</i>	[75058]
	28775.67	(0.10)	6(4, 3) - 6(3, 4)				[61014]
	28794.628	(0.030)	4(2, 3) - 4(1, 4)		<i>A₁A₂</i>	<i>1ν₁</i>	[75058]
	28799.251	(0.030)	4(2, 3) - 4(1, 4)		<i>EE</i>	<i>1ν₁</i>	[75058]
	28803.859	(0.030)	4(2, 3) - 4(1, 4)	<i>A₁</i>	<i>E + EA₂</i>	<i>1ν₁</i>	[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)		<i>EA</i>		[75058]
	29852.000	(0.030)	9(9, 1) - 9(8, 2)		<i>AE</i>		[75058]
	29852.580	(0.030)	9(9, 1) - 9(8, 2)		<i>EE</i>		[75058]
	29853.583	(0.030)	9(9, 1) - 9(8, 2)		<i>AA</i>		[75058]
	29908.76	(0.10)	14(12, 2) - 14(11, 3)		<i>AE + EA</i>		[61014]
	29909.89	(0.10)	14(12, 2) - 14(11, 3)		<i>EE</i>		[61014]
	29910.98	(0.10)	14(12, 2) - 14(11, 3)		<i>AA</i>		[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)		<i>AE</i>		[75058]
	31933.042	(0.030)	12(11, 1) - 12(10, 2)		<i>EA</i>		[75058]
	31933.956	(0.030)	12(11, 1) - 12(10, 2)		<i>EE</i>		[75058]
	31934.994	(0.030)	12(11, 1) - 12(10, 2)		<i>AA</i>		[75058]
	31937.872	(0.030)	17(14, 3) - 17(13, 4)		<i>AE + EA</i>		[75058]
	31938.959	(0.030)	17(14, 3) - 17(13, 4)		<i>EE</i>		[75058]
	31940.047	(0.030)	17(14, 3) - 17(13, 4)		<i>AA</i>		[75058]
	32015.95	(0.10)	2(2, 1) - 1(1, 0)				[61014]
	33291.123	(0.030)	10(10, 1) - 10(9, 2)		<i>EA</i>		[75058]
	33293.126	(0.030)	10(10, 1) - 10(9, 2)		<i>AE</i>		[75058]
	33293.497	(0.030)	10(10, 1) - 10(9, 2)		<i>EE</i>		[75058]
	33294.910	(0.030)	10(10, 1) - 10(9, 2)		<i>AA</i>		[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)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	$v_1 v_2$	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

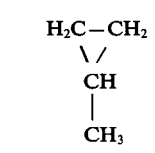
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	ν_t	Sym.	Ref.
CH ₂ CH ₂ CHCH ₃	11949.95	(0.05)	1(0, 1) - 0(0, 0)	0		[68048]
	16017.18	(0.05)	8(2, 7) - 8(1, 7)	0		[68048]
	20867.76	(0.05)	6(2, 5) - 6(1, 5)	0		[68048]
	21157.80	(0.05)	21(4, 18) - 21(3, 18)	0	<i>E</i>	[68048]
	21158.03	(0.05)	21(4, 18) - 21(3, 18)	0	<i>A</i>	[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	<i>E</i>	[68048]
	23551.11	(0.05)	27(5, 23) - 27(4, 23)	0	<i>A</i>	[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	<i>A</i>	[68048]
	25231.12	(0.05)	30(6, 24) - 30(6, 25)	0	<i>E</i>	[68048]
	25399.07	(0.05)	13(3, 11) - 13(2, 11)	0		[68048]
	25780.06	(0.05)	20(4, 17) - 20(3, 17)	0	<i>E</i>	[68048]
	25780.30	(0.05)	20(4, 17) - 20(3, 17)	0	<i>A</i>	[68048]
	30656.08	(0.05)	19(4, 16) - 19(3, 16)	0	<i>E</i>	[68048]
	30656.36	(0.05)	19(4, 16) - 19(3, 16)	0	<i>A</i>	[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_1 C_4H_8

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]
$\begin{array}{c} H_2C-CH_2 \\ \quad \\ H_2C-CHD \end{array}$	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]
	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]
α -CH ₂ CH ₂ CH ₂ CHD	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_o	(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)		
$q\ell(\tau_e)$	(MHz)	21.0		
$q\ell(\delta_e)$	(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]
	31162.95	(0.05)	2() - 1()		[60010]
$(\text{CH}_3)_3\text{CD}$	31162.95	(0.05)	2() - 1()		[60010]
	30426.24	(0.10)	2(1, 1) - 1(0, 1)		[60010]
$^{13}\text{CH}_3(\text{CH}_3)_2\text{CH}$	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]
	30031.28	(0.10)	2(2, 0) - 1(1, 0)		[60010]
sym- $\text{CH}_2\text{D}(\text{CH}_3)_2\text{CH}$	30266.06	(0.20)	2(2, 1) - 1(1, 1)		[60010]
	29560.45	(0.05)	2(1, 1) - 1(0, 1)		[60010]
	30147.92	(0.05)	2(2, 0) - 1(1, 0)		[60010]
asy- $\text{CH}_2\text{D}(\text{CH}_3)_2\text{CH}$	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)	1ν 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

C₅H₄

Isotopic species	Frequency (MHz)	Unc. (MHz)	J' K ₋₁ - J'' K ₊₁	Vib. state	Ref.
CH ₃ C ₄ 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

C₅H₄

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 ₂ 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 ₂ 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)×10 ⁻⁶ erg/(G ² ·mol)
2χ _{bb} -χ _{aa} -χ _{cc}	+37.8(3)×10 ⁻⁶ erg/(G ² ·mol)
Q _{aa}	1.4(4)×10 ⁻²⁶ esu·cm ²
Q _{bb}	3.7(4)×10 ⁻²⁶ esu·cm ²
Q _{cc}	-5.1(5)×10 ⁻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 C₃ 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]		
CH ₂ CH ¹³ CHCHCH	20755.44	(0.05)	2(0, 2) - 1(1, 1)	[65030]	
	21078.23	(0.05)	2(1, 2) - 1(0, 1)	[65030]	
CH ₂ ¹³ CHCHCHCH	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)	
<u>Dipole Moment</u> [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)
<u>Rotational Constants</u> [83051]			
$\overline{\text{CH}_2\text{CH}_2^{13}\text{CHCCH}}$ (1- ¹³ C)	15538.76(3604)	3350.53(2)	3190.99(2)
$\overline{\text{CH}_2^{13}\text{CH}_2\text{CHCCH}}$ (2- ¹³ C)	15426.69(2363)	3319.58(2)	3146.32(2)
$\overline{\text{CH}_2\text{CH}_2\text{CH}^{13}\text{CCH}}$ (4- ¹³ C)	15681.92(2400)	3334.68(2)	3170.33(2)
$\overline{\text{CH}_2\text{CH}_2\text{CHC}^{13}\text{CH}}$ (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 ∨ CH C CH	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]
		25872.90	(0.05)	4(1, 4) - 3(1, 3)	[72062]
		26193.97	(0.05)	4(0, 4) - 3(0, 3)	[72062]
		26209.56	(0.05)	4(2, 3) - 3(2, 2)	[72062]
		26214.59	(0.05)	4(3, 1) - 3(3, 0)	[72062]
		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	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_2=\text{CC}\equiv\text{CH} \end{array}$
<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 CH ₃ H ₂ C=CCCH	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]
	13567.9	(0.1)	2(0, 2) - 1(0, 1)	A	[69067]
	14680.8	(0.1)	4(2, 2) - 4(1, 3)	A	[69067]
	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)	$\times 10^{-6} \text{ erg}/(\text{G}^2 \cdot \text{mol})$
$-\chi_{aa} + 2\chi_{bb} - \chi_{cc}$	7.8(15)	$\times 10^{-6} \text{ erg}/(\text{G}^2 \cdot \text{mol})$
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]
HC=CH	33104.42	(0.10)	3(1, 3) - 2(1, 2)	[70064]
	34245.47	(0.10)	3(0, 3) - 2(0, 2)	[70064]
HC-CH	35202.53	(0.10)	3(2, 2) - 2(2, 1)	[70064]
∨	36159.53	(0.10)	3(2, 1) - 2(2, 0)	[70064]
CH ₂	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)	$J'(K_-,K_{+1}) - J''(K_-,K_{+1})$	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	$\text{CH}_2=\overset{\text{CH}_3}{\text{C}}\text{CH}=\text{CH}_2$
<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 R₆ = 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

C₅H₈

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} (C_3-C_4 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.
<i>g</i> -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)	1ν ₃₁	[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

C₅H₈

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 ₃₃	[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 ₃₃	[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

C₅H₈

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
t -CH(CHCH ₂)CH ₂ CH ₂	11885.44	(0.05)	2(1, 2) - 1(1, 1)		[74063]
	12004.64	(0.05)	2(0, 2) - 1(0, 1)		[74063]
$ \begin{array}{c} \text{H}_2\text{C}-\text{CH}_2 \\ \diagdown \\ \text{CH} \\ \\ \text{CH} \\ \\ \text{CH}_2 \end{array} $	12125.54	(0.05)	2(1, 1) - 1(1, 0)		[74063]
	17827.57	(0.05)	3(1, 3) - 2(1, 2)		[74063]
	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)	1ν ₃₃	[74063]
	12029.99	(0.05)	2(0, 2) - 1(0, 1)	1ν ₃₃	[74063]
	12158.41	(0.05)	2(1, 1) - 1(1, 0)	1ν ₃₃	[74063]
	24053.84	(0.05)	4(0, 4) - 3(0, 3)	1ν ₃₃	[74063]
	24060.90	(0.05)	4(2, 3) - 3(2, 2)	1ν ₃₃	[74063]
	29754.32	(0.05)	5(1, 5) - 4(1, 4)	1ν ₃₃	[74063]
	30057.05	(0.05)	5(0, 5) - 4(0, 4)	1ν ₃₃	[74063]
	30074.74	(0.05)	5(2, 4) - 4(2, 3)	1ν ₃₃	[74063]
	30095.08	(0.05)	5(2, 3) - 4(2, 2)	1ν ₃₃	[74063]
	30391.32	(0.05)	5(1, 4) - 4(1, 3)	1ν ₃₃	[74063]
	23840.84	(0.05)	4(1, 4) - 3(1, 3)	2ν ₃₃	[74063]
	29798.84	(0.05)	5(1, 5) - 4(1, 4)	2ν ₃₃	[74063]
	30117.72	(0.05)	5(0, 5) - 4(0, 4)	2ν ₃₃	[74063]
30137.72	(0.05)	5(2, 4) - 4(2, 3)	2ν ₃₃	[74063]	
30160.66	(0.05)	5(2, 3) - 4(2, 3)	2ν ₃₃	[74063]	
30472.21	(0.05)	5(1, 4) - 4(1, 3)	2ν ₃₃	[74063]	
29842.29	(0.05)	5(1, 5) - 4(1, 4)	3ν ₃₃	[74063]	
30177.06	(0.05)	5(0, 5) - 4(0, 4)	3ν ₃₃	[74063]	
30199.51	(0.05)	5(2, 4) - 4(2, 3)	3ν ₃₃	[74063]	
30225.19	(0.05)	5(2, 3) - 4(2, 2)	3ν ₃₃	[74063]	
t -CH(CHCH ₂) ¹³ CH ₂ 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)
CH ₂ CCH ₂ CH ₂ CH ₂				
<u>Rotational Constants</u> [68044]				
	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</u> [70063]				
g _{aa}		-0.0320(8)	μ _N	
g _{bb}		-0.0218(10)	μ _N	
g _{cc}		-0.0184(11)	μ _N	
2χ _{aa} -χ _{bb} -χ _{cc}		-6.4(5)x10 ⁻⁶	erg/(G ² ·mol)	
-χ _{aa} +2χ _{bb} -χ _{cc}		4.3(17)x10 ⁻⁶	erg/(G ² ·mol)	
Q _{aa}		-1.2(11)x10 ⁻²⁶	esu·cm ²	
Q _{bb}		-1.1(20)x10 ⁻²⁶	esu·cm ²	
Q _{cc}		2.3(24)x10 ⁻²⁶	esu·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]
	8066.56	(0.05)	1(0, 1) - 0(0, 0)		[68044]
H ₂ C-C=CH ₂	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]
H ₂ C-CH ₂	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]
	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]
	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]
	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]
	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]
	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]
	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]
	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]
	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]

TABLE 44.2. Microwave spectrum of methylene cyclobutane — Continued

C₃H₈

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

C₂H₆

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	
	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	(CH ₃) ₂ C=C=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)x10 ⁻³
Δ_{JK} (MHz)	0.010490(60)x10 ⁻³
Δ_K (MHz)	1.985(204)x10 ⁻³
δ_J (MHz)	0.15723(173)x10 ⁻³
δ_K (MHz)	6.108(40)x10 ⁻³
<u>Internal Rotation Constants [71050]</u>	
I_α (u Å 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)	
ν_{II}^a	8248.25(10)	3626.382(20)	2640.565(20)	~191.
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)	<i>EE</i>	1ν _I	[76060]
H ₃ C \ C=C=CH ₂	11523.34	(0.05)	14(4,10) - 14(4,11)	<i>EE</i>	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)	<i>EE</i>	1ν ₃₂	[77040]
	11564.87	(0.05)	2(1, 2) - 1(1, 1)	<i>EE</i>	1ν _I	[77040]
	11578.42	(0.05)	2(1, 2) - 1(1, 1)	<i>EE</i>	1ν _{II}	[77040]
	12014.68	(0.05)	12(4, 8) - 12(4, 9)	<i>EE</i>	1ν _I	[77040]
	12361.66	(0.05)	2(0, 2) - 1(0, 1)	<i>EE</i>	1ν _I	[77040]
	12365.69	(0.05)	2(0, 2) - 1(0, 1)	<i>A₂A₁</i>	1ν ₁₆	[77040]
	12366.03	(0.05)	2(0, 2) - 1(0, 1)	<i>EE</i>	1ν ₁₆	[77040]
	12366.44	(0.05)	2(0, 2) - 1(0, 1)	<i>AE + EA</i>	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)	<i>EE</i>	1ν ₃₂	[77040]
	12420.32	(0.05)	2(0, 2) - 1(0, 1)	<i>EE</i>	1ν _{II}	[77040]
	13462.64	(0.05)	2(1, 1) - 1(1, 0)	<i>EE</i>	1ν _I	[77040]
	13478.95	(0.05)	2(1, 1) - 1(1, 0)	<i>A₂A₁</i>	1ν ₁₆	[77040]
	13479.64	(0.05)	2(1, 1) - 1(1, 0)	<i>EE</i>	1ν ₁₆	[77040]
	13480.33	(0.05)	2(1, 1) - 1(1, 0)	<i>AE + EA</i>	1ν ₁₆	[77040]
	13481.98	(0.05)	2(1, 1) - 1(1, 0)			[71050]
	13493.08	(0.05)	2(1, 1) - 1(1, 0)	<i>EE</i>	1ν _{II}	[77040]
	13498.73	(0.05)	2(1, 1) - 1(1, 0)	<i>EE</i>	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)	<i>AE + EA</i>		[71050]
	13762.837	(0.080)	23(7,16) - 23(7,17)	<i>EE</i>		[71050]
	13763.368	(0.080)	23(7,16) - 23(7,17)	<i>AA</i>		[71050]
	14272.59	(0.05)	15(4,11) - 15(4,12)	<i>EE</i>	1ν _I	[77040]
	15419.158	(0.080)	20(6,14) - 20(6,15)	<i>AE + EA</i>		[71050]
	15419.661	(0.080)	20(6,14) - 20(6,15)	<i>EE</i>		[71050]
	15420.174	(0.080)	20(6,14) - 20(6,15)	<i>AA</i>		[71050]
	16034.36	(0.08)	10(2, 8) - 9(4, 5)			[76060]
	16459.89	(0.05)	8(2, 6) - 8(2, 7)	<i>EE</i>	1ν _{II}	[77040]
	16594.39	(0.05)	8(2, 6) - 8(2, 7)			[71050]
	16722.28	(0.05)	17(5,12) - 17(5,13)	<i>EE</i>	1ν ₃₂	[77040]
	16725.13	(0.05)	17(5,12) - 17(5,13)	<i>EE</i>	1ν ₃₂	[77040]
	16727.95	(0.05)	17(5,12) - 17(5,13)	<i>EE</i>	1ν ₃₂	[77040]
	16750.943	(0.080)	17(5,12) - 17(5,13)	<i>AE + EA</i>		[71050]
	16751.419	(0.080)	17(5,12) - 17(5,13)	<i>EE</i>		[71050]
	16751.890	(0.080)	17(5,12) - 17(5,13)	<i>AA</i>		[71050]
	16863.49	(0.05)	17(5,12) - 17(5,13)	<i>A₂A₁</i>	1ν ₁₆	[77040]
	16873.55	(0.05)	17(5,12) - 17(5,13)	<i>EE</i>	1ν ₁₆	[77040]
	16883.62	(0.05)	17(5,12) - 17(5,13)	<i>AE + EA</i>	1ν ₁₆	[77040]
	17033.113	(0.080)	37(11,26) - 37(11,27)	<i>AE + EA</i>		[71050]
	17033.969	(0.080)	37(11,26) - 37(11,27)	<i>EE</i>		[71050]
	17034.842	(0.080)	37(11,26) - 37(11,27)	<i>AA</i>		[71050]
	17212.02	(0.05)	3(1, 3) - 2(1, 2)	<i>A₂A₁</i>	1ν ₁₆	[77040]
	17212.31	(0.05)	3(1, 3) - 2(1, 2)	<i>EE</i>	1ν ₁₆	[77040]
	17212.62	(0.05)	3(1, 3) - 2(1, 2)	<i>AE + EA</i>	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)	<i>EE</i>	1ν ₃₂	[77040]
	17253.80	(0.05)	3(1, 3) - 2(1, 2)	<i>EE</i>	1ν _I	[77040]
	17269.87	(0.05)	3(1, 3) - 2(1, 2)	<i>AE + EA</i>	2ν ₃₂	[77040]
	17270.26	(0.05)	3(1, 3) - 2(1, 2)	<i>EE</i>	2ν ₃₂	[77040]
	17270.62	(0.05)	3(1, 3) - 2(1, 2)	<i>AA</i>	2ν ₃₂	[77040]
	17311.34	(0.05)	3(1, 3) - 2(1, 2)	<i>EE</i>	1ν _{II}	[77040]
	17525.60	(0.05)	14(4,10) - 14(4,11)	<i>EE</i>	1ν ₃₂	[77040]
	17528.02	(0.05)	14(4,10) - 14(4,11)	<i>EE</i>	1ν ₃₂	[77040]
	17530.49	(0.05)	14(4,10) - 14(4,11)	<i>EE</i>	1ν ₃₂	[77040]
	17547.544	(0.080)	14(4,10) - 14(4,11)	<i>AE + EA</i>		[71050]
	17547.940	(0.080)	14(4,10) - 14(4,11)	<i>EE</i>		[71050]
	17548.345	(0.080)	14(4,10) - 14(4,11)	<i>AA</i>		[71050]
	17564.23	(0.05)	11(3, 8) - 11(3, 9)	<i>EE</i>	1ν ₃₂	[77040]
	17566.20	(0.05)	11(3, 8) - 11(3, 9)	<i>EE</i>	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

C₃H₆

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

C₅H₈

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 _I	[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 _{II}	[77040]
	28958.60	(0.05)	5(0, 5) - 4(0, 4)	EE	1ν _I	[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 _{II}	[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 _I	[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 _I	[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 _I	[77040]
	31099.38	(0.05)	7(2, 6) - 7(0, 7)	EE	1ν _{II}	[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 _I	[77040]
	31625.75	(0.05)	5(3, 3) - 4(3, 2)			[71050]
	31650.13	(0.05)	5(3, 3) - 4(3, 2)	EE	1ν _{II}	[77040]
	31831.41	(0.05)	5(3, 2) - 4(3, 1)	EE	1ν _{II}	[77040]
	31835.50	(0.05)	5(2, 4) - 4(2, 3)	EE	1ν _{II}	[77040]
	31873.57	(0.05)	5(3, 2) - 4(3, 1)			[71050]
	31875.89	(0.05)	5(3, 2) - 4(3, 1)	EE	1ν _I	[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 _I	[77040]
	32391.44	(0.05)	6(3, 3) - 5(1, 5)		1ν _I → 1ν _{II}	[77040]
	32761.27	(0.05)	5(1, 4) - 4(1, 3)	EE	1ν _I	[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)

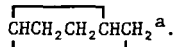
^aAssumed.

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 CHCHCHCH 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 CHCHCHCH 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]	
	32439.60	(0.05)	2(2, 0) - 1(1, 0)	[72064]	
¹³ CHCH ₂ CH ₂ CHCH ₂	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]	
	15039.08	(0.10)	1(1, 0) - 0(0, 0)	[72064]	
CH ¹³ CH ₂ CH ₂ CHCH ₂	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]	
	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]	
CHCH ₂ CH ₂ CH ¹³ CH ₂	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]	
	33159.87	(0.10)	2(2, 1) - 1(1, 1)	[72064]	
	CDCH ₂ CH ₂ CHCH ₂	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

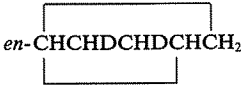
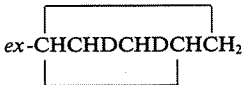
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
	27255.29	(0.02)	5(5, 1) - 5(4, 1)	[76052]
	27349.97	(0.02)	5(5, 0) - 5(4, 2)	[76052]
	29695.35	(0.02)	2(2, 0) - 1(1, 0)	[76052]
	30575.87	(0.02)	2(2, 1) - 1(1, 1)	[76052]
	33432.82	(0.02)	6(6, 1) - 6(5, 1)	[76052]
	35187.94	(0.02)	4(1, 3) - 3(2, 1)	[76052]
	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


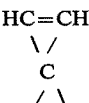
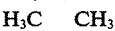
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
	27599.39	(0.10)	3(2, 2) - 2(2, 1)	[78029]
	29262.56	(0.10)	3(1, 2) - 2(1, 1)	[78029]
	29754.80	(0.10)	3(2, 1) - 2(2, 0)	[78029]
	32832.34	(0.10)	4(1, 4) - 3(1, 3)	[78029]
	33003.42	(0.10)	4(0, 4) - 3(0, 3)	[78029]
	36228.39	(0.10)	4(2, 3) - 3(2, 2)	[78029]
	37727.62	(0.10)	4(1, 3) - 3(1, 2)	[78029]
	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)	4v ₁	[62023]
	11745.61	(0.10)	10(10, 1) - 10(9, 2)	1v ₁	[62023]
	11779.34	(0.10)	9(9, 1) - 9(8, 2)	2v ₁	[62023]
	11829.37	(0.10)	10(10, 1) - 10(9, 2)	3v ₁	[62023]
	11895.80	(0.10)	10(10, 1) - 10(9, 2)		[62023]
	11898.44	(0.10)	10(10, 1) - 10(9, 2)	4v ₁	[62023]
	12008.90	(0.10)	24(23, 1) - 24(22, 2)		[62023]
	12115.24	(0.10)	11(11, 1) - 11(10, 2)	1v ₁	[62023]
	12185.58	(0.10)	10(10, 1) - 10(9, 2)	2v ₁	[62023]
	12213.43	(0.10)	11(11, 1) - 11(10, 2)	3v ₁	[62023]
	12293.54	(0.10)	11(11, 1) - 11(10, 2)		[62023]
	12294.98	(0.10)	11(11, 1) - 11(10, 2)	4v ₁	[62023]
	12519.77	(0.10)	12(12, 1) - 12(11, 2)	1v ₁	[62023]
	12633.75	(0.10)	12(12, 1) - 12(11, 2)	3v 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)	1v ₁	[62023]
	13089.93	(0.10)	13(13, 1) - 13(12, 2)	3v ₁	[62023]
	13124.13	(0.10)	12(12, 1) - 12(11, 2)	2v ₁	[62023]
	13198.7	(0.3)	13(13, 1) - 13(12, 2)		[62023]
	13434.97	(0.10)	14(14, 1) - 14(13, 2)	1v ₁	[62023]
	13581.78	(0.10)	14(14, 1) - 14(13, 2)	3v ₁	[62023]
	13656.2	(0.3)	13(13, 1) - 13(12, 2)	2v ₁	[62023]
	13705.1	(0.3)	14(14, 1) - 14(13, 2)		[62023]
	13706.6	(0.3)	14(14, 1) - 14(13, 2)	4v ₁	[62023]
	13944.1	(0.3)	15(15, 1) - 15(14, 2)	1v ₁	[62023]
	14108.7	(0.3)	15(15, 1) - 15(14, 2)	3v ₁	[62023]
	14228.7	(0.3)	14(14, 1) - 14(13, 2)	2v ₁	[62023]
	14246.2	(0.3)	15(15, 1) - 15(14, 2)		[62023]
	14487.50	(0.10)	16(16, 1) - 16(15, 2)	1v ₁	[62023]
	14670.75	(0.10)	16(16, 1) - 16(15, 2)	3v ₁	[62023]
	14820.90	(0.10)	16(16, 1) - 16(15, 2)		[62023]
	14828.7	(0.3)	16(16, 1) - 16(15, 2)	4v ₁	[62023]
	14841.1	(0.3)	15(15, 1) - 15(14, 2)	2v ₁	[62023]
	15063.75	(0.10)	17(17, 1) - 17(16, 2)	1v ₁	[62023]
	16324.8	(0.2)	9(7, 2) - 9(6, 3)	2v ₁	[65035]
	16329.6	(0.2)	9(7, 2) - 9(6, 3)	4v ₁	[65035]
	16409.7	(0.2)	8(6, 2) - 8(5, 3)	3v ₁	[65035]
	16415.9	(0.2)	8(6, 2) - 8(5, 3)	4v ₁	[65035]
	16431.8	(0.2)	8(6, 2) - 8(5, 3)	2v ₁	[65035]
	16468.73	(0.20)	7(5, 2) - 7(4, 3)	3v ₁	[65035]
	16478.10	(0.20)	7(5, 2) - 7(4, 3)	4v ₁	[65035]
	16509.25	(0.20)	6(4, 2) - 6(3, 3)	3v ₁	[65035]
	16520.45	(0.20)	6(4, 2) - 6(3, 3)	4v ₁	[65035]
	16527.03	(0.20)	7(5, 2) - 7(4, 3)	2v ₁	[65035]
	16534.53	(0.20)	5(3, 2) - 5(2, 3)	3v ₁	[65035]
	16557.05	(0.20)	3(1, 2) - 3(0, 3)	3v ₁	[65035]
	16562.28	(0.20)	6(4, 2) - 6(3, 3)	2v ₁	[65035]
	16563.15	(0.20)	3(2, 2) - 3(1, 3)	3v ₁	[65035]
	16564.88	(0.20)	4(3, 2) - 4(2, 3)	3v ₁	[65035]
	16570.40	(0.20)	5(4, 2) - 5(3, 3)	3v ₁	[65035]
	16580.10	(0.20)	6(3, 2) - 6(4, 3)	3v ₁	[65035]
	16595.8	(0.2)	7(6, 2) - 7(5, 3)	3v ₁	[65035]
	16596.10	(0.20)	5(3, 2) - 5(2, 3)	2v ₁	[65035]
	16612.9	(0.2)	7(6, 2) - 7(5, 3)	4v ₁	[65035]
	16615.78	(0.20)	4(2, 2) - 4(1, 3)	2v ₁	[65035]
	16625.68	(0.20)	3(1, 2) - 3(0, 3)	2v ₁	[65035]
	16632.95	(0.20)	3(2, 2) - 3(1, 3)	2v ₁	[65035]
	16636.48	(0.20)	4(3, 2) - 4(2, 3)	2v ₁	[65035]
	16644.20	(0.20)	5(4, 2) - 5(3, 3)	2v ₁	[65035]
	16657.68	(0.20)	6(5, 2) - 5(4, 3)	2v ₁	[65035]
	16679.2	(0.2)	7(6, 2) - 7(5, 3)	2v ₁	[65035]
	18948.8	(0.2)	2(0, 2) - 1(1, 1)	2v ₁	[65035]
	19028.70	(0.20)	2(1, 2) - 1(0, 1)	2v ₁	[65035]
	19036.35	(0.20)	2(0, 2) - 1(1, 1)	3v ₁	[65035]
	19073.50	(0.10)	2(0, 2) - 1(1, 1)		[62023]
	19080.86	(0.10)	2(0, 2) - 1(1, 1)	1v 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,
 $(\text{CH}_3)_2\overset{\text{I}}{\text{C}}\text{CH}_2\text{CH}_2$.

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 R₆ = 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]
$ \begin{array}{c} \text{H}_2\text{C}-\text{CH}_2 \\ \diagdown \quad / \\ \text{C} \\ / \quad \backslash \\ \text{CH}_3 \quad \text{CH}_3 \end{array} $	28373.19	(0.05)	3(1, 2) - 2(1, 1)	[79031]
	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	$v_{39} = 1$	$v_{39} = 2$	$v_{39} = 3$
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	$v_{39} = 1^d$	$v_{39} = 2^d$
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 Å 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)	$J'(K_{-1}, K_{-1}) - J''(K_{+1}, K_{+1})$	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

C₃H₁₀

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

TABLE 53.3. Microwave spectrum of 2-pentene — Continued

C₅H₁₀

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-i}, K_{-i}) - J''(K_{+i}, K_{+i})$	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	<i>A</i>	[81037]
	38414.00	(0.10)	15(2,13) - 14(3,12)	0	<i>A</i>	[81037]
	38442.08	(0.10)	15(2,13) - 14(3,12)	0	<i>E</i>	[81037]
	38535.41	(0.10)	24(2,22) - 24(1,23)	0	<i>E</i>	[81037]
	38648.49	(0.10)	24(2,22) - 24(1,23)	0	<i>A</i>	[81037]
	40286.60	(0.10)	7(1, 7) - 6(0, 6)	0	<i>A</i>	[81037]
	40287.08	(0.10)	7(1, 7) - 6(0, 6)	0	<i>E</i>	[81037]
	40444.04	(0.10)	7(1, 7) - 6(0, 6)	1	<i>A</i>	[81037]
	40444.16	(0.10)	7(1, 7) - 6(0, 6)	1	<i>E</i>	[81037]
	40594.36	(0.10)	15(2,13) - 4(3,12)	1	<i>A</i>	[81037]
	40613.06	(0.10)	15(2,13) - 3,12)	1	<i>E</i>	[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 Π _{3/2}	20792.872	(0.020)	15/2 - 13/2	<i>f</i>	8 - 7	$v = 0$	[87007]	
	20792.944	(0.020)	15/2 - 13/2	<i>f</i>	7 - 6	$v = 0$	[87007]	
	20794.441	(0.020)	15/2 - 13/2	<i>e</i>	8 - 7	$v = 0$	[87007]	
	20794.511	(0.020)	15/2 - 13/2	<i>e</i>	7 - 6	$v = 0$	[87007]	
	23565.160	(0.020)	17/2 - 15/2	<i>f</i>	9 - 8	$v = 0$	[86022]	
	23565.226	(0.020)	17/2 - 15/2	<i>f</i>	8 - 7	$v = 0$	[86022]	
	23567.169	(0.020)	17/2 - 15/2	<i>e</i>	9 - 8	$v = 0$	[86022]	
	23567.238	(0.020)	17/2 - 15/2	<i>e</i>	8 - 7	$v = 0$	[86022]	
	40198.356	(0.030)	29/2 - 27/2	<i>f</i>		$v = 0$	[86022]	
	40204.150	(0.030)	29/2 - 27/2	<i>e</i>		$v = 0$	[86022]	
	42970.453	(0.030)	31/2 - 29/2	<i>f</i>		$v = 0$	[86022]	
	42977.115	(0.020)	31/2 - 29/2	<i>e</i>		$v = 0$	[86022]	
	73460.	(1.0)	53/2 - 51/2	<i>f</i>		$v = 0$	[87007]	
	73480.5	(1.0)	53/2 - 51/2	<i>e</i>		$v = 0$	[87007]	
	81778.1	(0.3)	59/2 - 57/2	<i>f</i>		$v = 0$	[87007]	
	81801.1	(0.3)	59/2 - 57/2	<i>e</i>		$v = 0$	[87007]	
	84549.9	(0.4)	61/2 - 59/2	<i>f</i>		$v = 0$	[87007]	
	84574.5	(0.5)	61/2 - 59/2	<i>e</i>		$v = 0$	[87007]	
	87348.3	(0.5)	63/2 - 61/2	<i>e</i>		$v = 0$	[87007]	
	90093.0	(0.4)	65/2 - 63/2	<i>f</i>		$v = 0$	[87007]	
	90121.4	(0.5)	65/2 - 63/2	<i>e</i>		$v = 0$	[87007]	
	92865.2	(0.3)	67/2 - 65/2	<i>f</i>		$v = 0$	[87007]	
	92894.9	(0.3)	67/2 - 65/2	<i>e</i>		$v = 0$	[87007]	
	95636.6	(0.3)	69/2 - 67/2	<i>f</i>		$v = 0$	[87007]	
	95668.3	(0.6)	69/2 - 67/2	<i>e</i>		$v = 0$	[87007]	
	98408.9	(0.4)	71/2 - 69/2	<i>f</i>		$v = 0$	[87007]	
	98441.7	(0.5)	71/2 - 69/2	<i>e</i>		$v = 0$	[87007]	
	101180.3	(0.3)	72/2 - 71/2	<i>f</i>		$v = 0$	[87009]	
	101251.9	(1.5)	72/2 - 71/2	<i>e</i>		$v = 0$	[87009]	
	103951.9	(0.4)	75/2 - 73/2	<i>f</i>		$v = 0$	[87009]	
	103989.0	(0.4)	75/2 - 73/2	<i>e</i>		$v = 0$	[87009]	
	106762.7	(0.3)	75/2 - 75/2	<i>e</i>		$v = 0$	[87009]	
	115038.4	(0.7)	83/2 - 81/2	<i>f</i>		$v = 0$	[87009]	
	115084.0	(0.7)	83/2 - 81/2	<i>e</i>		$v = 0$	[87009]	
	CCCCCCH ² Π _{1/2}	43261.60	(0.30)	31/2 - 29/2	<i>f</i>		$v = 0$	[87006]
		43294.60	(0.30)	31/2 - 29/2	<i>e</i>		$v = 0$	[87006]
		73967.00	(0.30)	53/2 - 51/2	<i>f</i>		$v = 0$	[86024]
		74008.00	(0.30)	53/2 - 51/2	<i>e</i>		$v = 0$	[86024]
		82384.5	(0.5)	59/2 - 57/2	<i>e</i>		$v = 0$	[87009]
		85131.1	(0.4)	61/2 - 59/2	<i>f</i>		$v = 0$	[87009]
		85176.0	(0.4)	61/2 - 59/2	<i>e</i>		$v = 0$	[87009]
		87921.7	(0.3)	63/2 - 61/2	<i>f</i>		$v = 0$	[87009]
		87967.7	(0.3)	63/2 - 61/2	<i>e</i>		$v = 0$	[87009]
90712.2		(0.3)	65/2 - 63/2	<i>f</i>		$v = 0$	[87009]	
90759.3		(0.3)	65/2 - 63/2	<i>e</i>		$v = 0$	[87009]	
93502.2		(1.0)	67/2 - 65/2	<i>f</i>		$v = 0$	[87009]	
93550.9		(0.5)	67/2 - 65/2	<i>e</i>		$v = 0$	[87009]	
96293.3		(0.3)	69/2 - 67/2	<i>f</i>		$v = 0$	[87006]	
96342.5		(0.3)	69/2 - 67/2	<i>e</i>		$v = 0$	[87006]	
99083.9		(0.3)	71/2 - 69/2	<i>f</i>		$v = 0$	[87006]	
99134.1		(0.3)	71/2 - 69/2	<i>e</i>		$v = 0$	[87006]	
101873.6		(1.0)	73/2 - 71/2	<i>f</i>		$v = 0$	[87009]	
101925.2		(0.7)	73/2 - 71/2	<i>e</i>		$v = 0$	[87009]	
107453.2		(0.3)	77/2 - 75/2	<i>f</i>		$v = 0$	[87009]	
107507.9		(0.4)	77/2 - 75/2	<i>e</i>		$v = 0$	[87009]	
110229.8		(1.0)	79/2 - 77/2	<i>e</i>		$v = 0$	[87009]	
110243.4		(1.0)	79/2 - 77/2	<i>f</i>		$v = 0$	[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.	
CHCHC(CH ₂)C(CH ₂)	19123.19	(0.05)	2(2, 1) - 1(1, 0)	[83033]	
	19601.66	(0.05)	7(5, 3) - 7(4, 4)	[83033]	
H ₂ C=C-C=CH ₂ HC=CH	21467.28	(0.05)	7(4, 4) - 7(3, 5)	[83033]	
	21656.01	(0.05)	4(0, 4) - 3(1, 3)	[83033]	
13CHCHC(CH ₂)C(CH ₂)	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]	
	CHCH ¹³ C(CH ₂)C(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]	
CHCH ¹³ C(CH ₂)C(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]
	39120.94	(0.05)	5(3, 3) - 4(2, 2)	[83033]
CDCDC(CH ₂)C(CH ₂)	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>e</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.	
CHCHCHCHCHCH	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]	
	¹³ CHCHCHCHCHCH	36268.079	(0.050)	4(2, 3) - 3(2, 2)	[72067]
		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]	
CH ¹³ CHCHCHCHCH	35843.07	(0.05)	4(2, 3) - 3(2, 2)	[73076]	
	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]	
	36793.90	(0.05)	4(3, 2) - 3(3, 1)	[73076]	
	CDCHCHCHCHCH	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]	
18355.81		(0.05)	5(3, 3) - 5(1, 4)	[73076]	
18130.33		(0.05)	5(2, 4) - 5(0, 5)	[73076]	
CHCDCHCHCHCH	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]	
	36952.09	(0.05)	4(3, 2) - 3(3, 1)	[73076]	
	17049.68	(0.05)	5(3, 3) - 5(1, 4)	[73076]	
CHCHCDCHCHCH	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

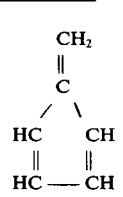
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.	
$\text{C}(\text{CH}_2)\text{CHCHCHCH}$ 	6399.18	(0.04)	1(0, 1) - 0(0, 0)	[72066]	
	11592.09	(0.04)	2(1, 2) - 1(1, 1)	[72066]	
	12581.87	(0.04)	2(0, 2) - 1(0, 1)	[72066]	
	14004.66	(0.04)	2(1, 1) - 1(1, 0)	[72066]	
	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 C(CH ₂)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]
C(CH ₂) ¹³ 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]	
C(CH ₂)CH ¹³ 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]	
	25085.42	(0.04)	4(2, 3) - 3(2, 2)	[72066]	
	33539.47	(0.04)	6(0, 5) - 5(0, 5)	[72066]	
C(¹³ CH ₂)CHCHCHCH	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]	
	13577.60	(0.04)	2(1, 1) - 1(1, 0)	[72066]	
	16832.04	(0.04)	3(1, 3) - 2(1, 2)	[72066]	
C(CH ₂)CDCHCHCH	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]	
	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]	
C(CH ₂)CHCDCHCH	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</u> [74064]	
μ_c (D)	0.0437

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

C₆H₆

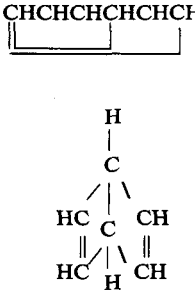
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
	20385.68	(0.10)	8(4, 5) - 8(3, 5)	[74064]
	21208.35	(0.10)	2(1, 1) - 1(0, 1)	[74064]
	26527.39	(0.10)	5(0, 5) - 4(1, 3)	[74064]
	26992.00	(0.10)	2(2, 0) - 1(1, 0)	[74064]
	27457.11	(0.10)	7(3, 4) - 7(2, 6)	[74064]
	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

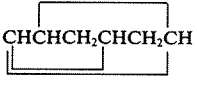
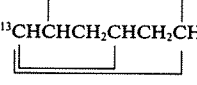
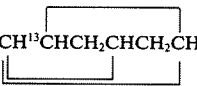
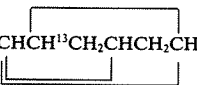
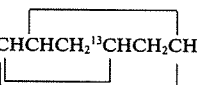
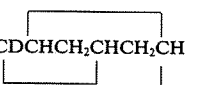
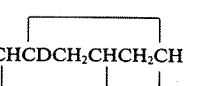
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.	
	11210.47	(0.05)	1(1, 0) - 0(0, 0)	[75051]	
	18477.29	(0.05)	2(1, 2) - 1(0, 1)	[75051]	
	21723.27	(0.05)	2(1, 1) - 1(0, 1)	[75051]	
	22036.64	(0.05)	2(2, 1) - 1(1, 0)	[75051]	
	22665.63	(0.05)	2(2, 0) - 1(1, 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)
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

C₆H₈

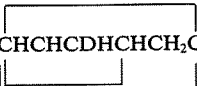

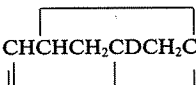
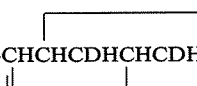
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.	
$en\text{-CHCHCDHCHCH}_2\text{CH}_8$ 	23071.67	(0.05)	2(2, 0) - 1(1, 1)	[75051]	
	25379.15	(0.05)	3(0, 3) - 2(1, 2)	[75051]	
	20993.57	(0.05)	2(1, 1) - 1(0, 1)	[75051]	
	21928.58	(0.05)	2(2, 0) - 1(1, 0)	[75051]	
	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]	
	$ex\text{-CHCHCHDCHCH}_2\text{CH}$ 	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]	
$CHCHCH_2CDCH_2CH$ 		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]	
	$en\text{-CHCHCDHCHCDHCH}$ 	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


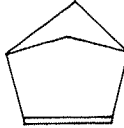
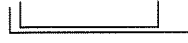
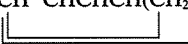

Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
$\text{CHCHCHCH}(\text{CH}_2)\text{CH}_2$  	8979.22	(0.05)	1(0, 1) - 0(0, 0)	[76054]
	17558.43	(0.05)	2(1, 2) - 1(1, 1)	[76054]
	17869.75	(0.05)	2(0, 2) - 1(0, 1)	[76054]
	26287.22	(0.05)	3(1, 3) - 2(1, 2)	[76054]
	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]
$^{13}\text{CHCHCHCH}(\text{CH}_2)\text{CH}_2$ 	36552.66	(0.05)	4(2, 2) - 3(2, 1)	[76054]
	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]
$\text{CH}^{13}\text{CHCHCH}(\text{CH}_2)\text{CH}_2$ 	36482.44	(0.05)	4(2, 2) - 3(2, 1)	[76054]
	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)
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


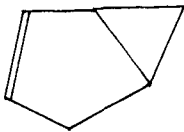
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.	
$\text{CHCHCHCH}_2\text{CHCH}_2$  	20543.37	(0.05)	3(0, 3) - 2(1, 2)	[78030]	
	20944.57	(0.05)	3(1, 3) - 2(1, 2)	[78030]	
	21925.66	(0.05)	3(1, 3) - 2(0, 2)	[78030]	
	22626.70	(0.05)	2(2, 0) - 1(1, 0)	[78030]	
	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 CHCHCHCH ₂ 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]	
CH ¹³ CHCHCH ₂ 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]	
CHCHCHCH ₂ ¹³ 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]	
CHCHCHCH ₂ CH ¹³ CH ₂	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]	
H ₂ C=C-C=CH ₂ H ₂ C-CH ₂	29378.76	(0.05)	5(1, 4) - 4(2, 3)		[75052]	
	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

C₆H₈

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]		
v State	B _v (MHz)	q _v (MHz)
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 _{Te} ℓ = -1	[62022]
	21453.5	(0.1)	4() - 3()	1ν _{Te}	[62022]
	21456.4	(0.1)	4() - 3()	1ν _{Ta}	[62022]
	21465.5	(0.1)	4() - 3()		[60008]
	21486.4	(0.1)	4() - 3()		[62022]
	21499.7	(0.1)	4(1) - 3(1)	1ν _{Be} ℓ = +1	[62022]
	26807.3	(0.1)	5(-1) - 4(-1)	1ν _{Te} ℓ = -1	[62022]
	26816.8	(0.1)	5() - 4()	1ν _{Te}	[62022]
	26820.4	(0.1)	5() - 4()	1ν _{Ta}	[62022]
	26831.9	(0.1)	5() - 4()		[62022]
	26857.7	(0.1)	5() - 4()		[62022]
	26874.5	(0.1)	5(1) - 4(1)	1ν _{Be} ℓ = +1	[62022]
	32168.4	(0.1)	6(-1) - 5(-1)	1ν _{Te} ℓ = -1	[62022]
	32179.8	(0.1)	6() - 5()	1ν _{Te}	[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) ₃ 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]
	20833.80	(0.08)	3(2, 2) - 2(1, 1)		[68046]
CDCDCD ₂ CD ₂ CD ₂ CD ₂	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

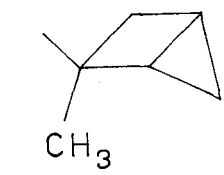
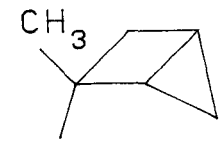
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J''(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
$en\text{-CHCH}(\text{CH}_3)\text{CH}_2\text{CHCH}_2$ 	27923.83	(0.10)	6(5, 2) - 6(4, 2)	[75053]
	28007.20	(0.10)	5(5, 0) - 5(4, 2)	[75053]
	29008.77	(0.10)	3(2, 2) - 2(1, 2)	[75053]
	31145.06	(0.10)	4(1, 3) - 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]

Electric Dipole Moment [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]
$\begin{array}{c} \text{H}_2\text{C}-\text{C}=\text{CH}_2 \\ \quad \\ \text{H}_2\text{C} \quad \text{CH}_2 \\ \backslash / \\ \text{CH}_2 \end{array}$	21761.67	(0.03)	9(2, 7) - 9(2, 8)		[72068]
	22293.33	(0.03)	4(2, 3) - 3(2, 2)		[72068]
	22702.16	(0.03)	4(3, 2) - 3(3, 1)		[72068]
	22814.13	(0.03)	4(3, 1) - 3(3, 0)		[72068]
	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

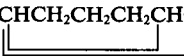
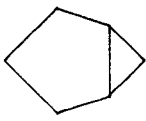
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
CHCH ₂ CH ₂ CH ₂ CHCH ₂ 	26577.31	(0.05)	4(1, 4) - 3(1, 3)	[74065]
	26748.10	(0.05)	4(0, 4) - 3(0, 3)	[74065]
	27362.41	(0.05)	3(1, 2) - 2(0, 2)	[74065]
	27973.74	(0.05)	3(2, 1) - 2(1, 1)	[74065]
	29075.87	(0.05)	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) ₂ 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)	1ν ₁₇ ℓ = -1	[78034]	
38955.28	(0.05)	25(7) - 24(7)	1ν ₁₇ ℓ = +1	[78034]	
38957.47	(0.05)	25(1) - 24(1)	1ν ₁₇ ℓ = +1	[78034]	
38957.48	(0.05)	25(4) - 24(4)	1ν ₁₇ ℓ = -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_l	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) - 9(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_t	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_t	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_i	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 $R_6 = 0$.^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

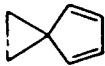
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
$\text{CH}_2\text{CH}_2\text{CCHCHCHCH}$ 	26741.50	(0.05)	6(2, 5) - 5(2, 4)	[81040]
	26986.17	(0.05)	6(5, 1) - 5(5, 0)	[81040]
	26986.17	(0.05)	6(5, 2) - 5(5, 1)	[81040]
	27003.15	(0.05)	12(1,11) - 12(1,12)	[81040]
	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 CH ₂ CH ₂ 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 CCHDCCH	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.
$\text{CH}(\text{CH}_2)\text{CHCHCHCH}_2\text{CH}_2$ 	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 R₆ = 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)	$J'(K_{-1}, K_{+1})$	-	$J''(K_{-1}, K_{+1})$	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)	$J'(K_{-1}, K_{+1})$	$J''(K_{-1}, K_{+1})$	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^{-13}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)		1ν <i>tw</i>	[79035]
	26798.14	(0.05)	5(2, 4) - 4(2, 3)		1ν <i>tw</i>	[79035]
	28999.64	(0.05)	5(2, 3) - 4(2, 2)		1ν <i>tw</i>	[79035]
	27666.42	(0.05)	5(3, 3) - 4(3, 2)		1ν <i>tw</i>	[79035]
	28378.54	(0.05)	5(3, 2) - 4(3, 1)		1ν <i>tw</i>	[79035]
	27735.53	(0.05)	5(4, 2) - 4(4, 1)		1ν <i>tw</i>	[79035]
27788.66	(0.05)	5(4, 1) - 4(4, 0)		1ν <i>tw</i>	[79035]	
29724.88	(0.05)	6(0, 6) - 5(0, 5)		1ν <i>tw</i>	[79035]	
29682.00	(0.05)	6(1, 6) - 5(1, 5)		1ν <i>tw</i>	[79035]	
32442.87	(0.05)	6(1, 5) - 5(1, 4)		1ν <i>tw</i>	[79035]	
31818.73	(0.05)	6(2, 5) - 5(2, 4)		1ν <i>tw</i>	[79035]	
34593.07	(0.05)	6(2, 4) - 5(2, 3)		1ν <i>tw</i>	[79035]	
33096.67	(0.05)	6(3, 4) - 5(3, 3)		1ν <i>tw</i>	[79035]	
34547.30	(0.05)	6(3, 3) - 5(3, 2)		1ν <i>tw</i>	[79035]	
33377.39	(0.05)	6(4, 3) - 5(4, 2)		1ν <i>tw</i>	[79035]	
33597.93	(0.05)	6(4, 2) - 5(4, 1)		1ν <i>tw</i>	[79035]	
33270.55	(0.05)	6(5, 2) - 5(5, 1)		1ν <i>tw</i>	[79035]	
33280.57	(0.05)	6(5, 1) - 5(5, 0)		1ν <i>tw</i>	[79035]	
34458.90	(0.05)	7(0, 7) - 6(0, 6)		1ν <i>tw</i>	[79035]	
34443.40	(0.05)	7(1, 7) - 6(1, 6)		1ν <i>tw</i>	[79035]	
37063.01	(0.05)	7(1, 6) - 6(1, 5)		1ν <i>tw</i>	[79035]	
36726.57	(0.05)	7(2, 6) - 6(2, 5)		1ν <i>tw</i>	[79035]	
39809.32	(0.05)	7(2, 5) - 6(2, 4)		1ν <i>tw</i>	[79035]	
39391.89	(0.05)	7(3, 5) - 6(3, 4)		1ν <i>tw</i>	[79035]	
38999.00	(0.05)	7(4, 4) - 6(4, 3)		1ν <i>tw</i>	[79035]	
39629.19	(0.05)	7(4, 3) - 6(4, 2)		1ν <i>tw</i>	[79035]	
38941.73	(0.05)	7(5, 3) - 6(5, 2)		1ν <i>tw</i>	[79035]	
38993.25	(0.05)	7(5, 2) - 6(5, 1)		1ν <i>tw</i>	[79035]	
39202.45	(0.05)	8(0, 8) - 7(0, 7)		1ν <i>tw</i>	[79035]	
39197.25	(0.05)	8(1, 8) - 7(1, 7)		1ν <i>tw</i>	[79035]	
27661.63	(0.05)	5(1, 4) - 4(1, 3)		1ν <i>pu</i>	[79035]	
28946.96	(0.05)	5(2, 3) - 4(2, 2)		1ν <i>pu</i>	[79035]	
27613.59	(0.05)	5(3, 3) - 4(3, 2)		1ν <i>pu</i>	[79035]	
28319.60	(0.05)	5(3, 2) - 4(3, 1)		1ν <i>pu</i>	[79035]	
27680.90	(0.05)	5(4, 2) - 4(4, 1)		1ν <i>pu</i>	[79035]	
27733.33	(0.05)	5(4, 1) - 4(4, 0)		1ν <i>pu</i>	[79035]	
29666.20	(0.05)	6(0, 6) - 5(0, 5)		1ν <i>pu</i>	[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 R_e = 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 (ν_1, ν_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 ν_1 and ring twisting vibration is ν_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

C₈H₆

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]
C(CCH)CH ¹³ CHCHCHCH	35605.56	(0.15)	13(10, 3) - 12(10, 2)	[75054]
	35622.83	(0.15)	13(9, 4) - 12(9, 3)	[75054]
	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]
$v_{4_2} = 1$	3654.53(59)	2008.489(56)	1302.525(99)	[76055]
$v_{4_2} = 2$	3640.46(95)	2012.436(96)	1307.64(10)	[76055]
$v_{4_2} = 3$	3620.9(1.3)	2015.72(25)	1313.47(27)	[76055]
$v_{4_2} = 4$	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

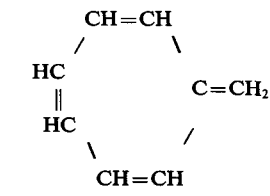
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
$C(CH_2)CHCHCHCHCHCH$	26997.75	(0.05)	8(7, 2) - 7(7, 1)		[76055]
	27121.35	(0.05)	8(6, 3) - 7(6, 2)		[76055]
	27125.91	(0.05)	8(6, 2) - 7(6, 1)		[76055]
	27303.05	(0.05)	8(4, 5) - 7(4, 4)		[76055]
	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>				
CH ₃ C ₆ H ₄ CH ₃	3163.930(50)	2150.069(5)	1300.835(5)	519.(3)
sym-CH ₂ DC ₆ H ₄ CH ₃	3045.778(100)	2123.611(10)	1271.100(10)	528.(9)
asy-CDH ₂ C ₆ H ₄ CH ₃	3123.019(100)	2089.736(10)	1276.442(10)	521.(8)
sym-CD ₂ HC ₆ H ₄ CH ₃	3085.147(100)	2032.070(10)	1253.577(10)	527.(8)
asy-CHD ₂ C ₆ H ₄ CH ₃	3014.161(100)	2062.862(10)	1248.191(10)	474.(13)
CD ₃ C ₆ H ₄ CH ₃	2984.204(100)	2005.184(10)	1226.690(10)	560.(24)
¹³ CH ₃ C ₆ H ₄ CH ₃	3123.542(50)	2119.462(5)	1282.807(5)	518.(6)
3d ₁ -CH ₃ C ₆ DH ₃ CH ₃	3048.552(50)	2145.490(10)	1279.293(5)	518.(11)
4d ₁ -CH ₃ C ₆ H ₃ 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)₄CCH₃

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>A</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]
	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]
C(¹³ CH ₃)(CH) ₄ CCH ₃	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)	<i>E</i> ₁₀	[73086]
	11976.72	(0.05)	25(12,13)	- 25(12,14)	<i>E</i> ₀₁	[73086]
	11977.59	(0.05)	25(12,13)	- 25(12,14)	<i>E</i> ₁₋₁	[73086]
	11977.59	(0.05)	25(12,13)	- 25(12,14)	<i>E</i> ₁₁	[73086]
	12044.79	(0.05)	33(16,17)	- 33(16,18)	<i>A</i>	[73086]
	12046.16	(0.05)	33(16,17)	- 33(16,18)	<i>E</i> ₁₀	[73086]
	12046.90	(0.05)	33(16,17)	- 33(16,18)	<i>E</i> ₀₁	[73086]
	12048.14	(0.05)	33(16,17)	- 33(16,18)	<i>E</i> ₁₋₁	[73086]
	12048.37	(0.05)	33(16,17)	- 33(16,18)	<i>E</i> ₁₁	[73086]
	12078.37	(0.05)	27(13,14)	- 27(13,15)	<i>A</i>	[73086]
	12079.37	(0.05)	27(13,14)	- 27(13,15)	<i>E</i> ₁₀	[73086]
	12079.92	(0.05)	27(13,14)	- 27(13,15)	<i>E</i> ₀₁	[73086]
	12080.90	(0.05)	27(13,14)	- 27(13,15)	<i>E</i> ₁₋₁	[73086]
	12080.90	(0.05)	27(13,14)	- 27(13,15)	<i>E</i> ₁₁	[73086]
	12108.26	(0.05)	31(15,16)	- 31(15,17)	<i>A</i>	[73086]
	12109.47	(0.05)	31(15,16)	- 31(15,17)	<i>E</i> ₁₀	[73086]
	12110.10	(0.05)	31(15,16)	- 31(15,17)	<i>E</i> ₀₁	[73086]
	12111.32	(0.05)	31(15,16)	- 31(15,17)	<i>E</i> ₁₋₁	[73086]
	12111.47	(0.05)	31(15,16)	- 31(15,17)	<i>E</i> ₁₁	[73086]
	12120.98	(0.05)	29(14,15)	- 29(14,16)	<i>A</i>	[73086]
	12122.09	(0.05)	29(14,15)	- 29(14,16)	<i>E</i> ₁₀	[73086]
	12122.70	(0.05)	29(14,15)	- 29(14,16)	<i>E</i> ₀₁	[73086]
	12123.82	(0.05)	29(14,15)	- 29(14,16)	<i>E</i> ₁₋₁	[73086]
	12123.82	(0.05)	29(14,15)	- 29(14,16)	<i>E</i> 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)	<i>A</i>	[73086]
	12628.22	(0.05)	26(13,13)	- 26(13,14)	<i>E</i> ₁₀	[73086]
	12628.57	(0.05)	26(13,13)	- 26(13,14)	<i>E</i> ₀₁	[73086]
	12629.63	(0.05)	26(13,13)	- 26(13,14)	<i>E</i> ₁₋₁	[73086]
	12629.63	(0.05)	26(13,13)	- 26(13,14)	<i>E</i> ₁₁	[73086]
	13249.18	(0.05)	28(14,14)	- 28(14,15)	<i>A</i>	[73086]
	13250.29	(0.05)	28(14,14)	- 28(14,15)	<i>E</i> ₁₀	[73086]
	13250.86	(0.05)	28(14,14)	- 28(14,15)	<i>E</i> ₀₁	[73086]
	13252.02	(0.05)	28(14,14)	- 28(14,15)	<i>E</i> ₁₋₁	[73086]
	13252.02	(0.05)	28(14,14)	- 28(14,15)	<i>E</i> 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)	<i>A</i>	[73086]
	14431.04	(0.05)	32(16,16)	- 32(16,17)	<i>E</i> ₁₀	[73086]
	14431.56	(0.05)	32(16,16)	- 32(16,17)	<i>E</i> ₀₁	[73086]
	14433.03	(0.05)	32(16,16)	- 32(16,17)	<i>E</i> ₁₋₁	[73086]
	14433.03	(0.05)	32(16,16)	- 32(16,17)	<i>E</i> ₁₁	[73086]
	14989.51	(0.05)	34(17,17)	- 34(17,18)	<i>A</i>	[73086]
	14991.13	(0.05)	34(17,17)	- 34(17,18)	<i>E</i> ₁₀	[73086]
	14991.78	(0.05)	34(17,17)	- 34(17,18)	<i>E</i> ₀₁	[73086]
	15513.190	(0.030)	4(2, 2)	- 3(2, 1)		[73086]
	15530.59	(0.05)	36(18,18)	- 36(18,19)	<i>A</i>	[73086]
	15532.58	(0.05)	36(18,18)	- 36(18,19)	<i>E</i> ₁₀	[73086]
	15533.15	(0.05)	36(18,18)	- 36(18,19)	<i>E</i> ₀₁	[73086]
	15534.82	(0.05)	36(18,18)	- 36(18,19)	<i>E</i> ₁₋₁	[73086]
	15534.82	(0.05)	36(18,18)	- 36(18,19)	<i>E</i> 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

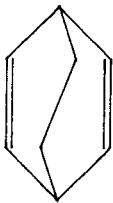
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
CHCHCHCHCHCH ₂ CH ₂	26656.46	(0.05)	5(1, 4) - 4(0, 4)	[83059]
	26669.20	(0.05)	5(2, 3) - 4(1, 3)	[83059]
	26770.07	(0.05)	5(2, 4) - 4(1, 4)	[83059]
	26840.26	(0.05)	5(3, 2) - 4(2, 2)	[83059]
	26872.65	(0.05)	5(3, 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

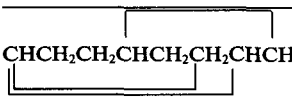
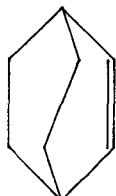
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
$\text{CHCH}_2\text{CH}_2\text{CHCH}_2\text{CH}_2\text{CHCH}$ 	30293.93	(0.05)	6(3, 3) - 5(2, 3)	[83059]
	30313.10	(0.05)	6(2, 4) - 5(1, 4)	[83059]
	30393.53	(0.05)	6(1, 5) - 5(0, 5)	[83059]
	30408.65	(0.05)	6(2, 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]	$\nu_{5,4} = 1^a$	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

C₈H₁₂

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)		[80036]
		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


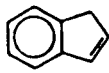
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Ref.
$\text{CH}_2\text{CHCHC}(\text{CH})_4\text{C}$ 	21289.48	(0.10)	9(1, 9) - 8(1, 8)	[79036]
	21329.78	(0.10)	9(0, 9) - 8(0, 8)	[79036]
	23542.28	(0.10)	10(1,10) - 9(1, 9)	[79036]
	23562.72	(0.10)	10(0,10) - 9(0, 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)
ν_6 (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
---------------	-------------

TABLE 88.3. Microwave spectrum of azulene

C₁₀H₈

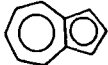
Isotopic species	Frequency (MHz)	Unc. (MHz)	$J'(K_{-1}, K_{+1}) - J''(K_{-1}, K_{+1})$	Vib. state	Ref.
CHCHCHC(CH) ₅ C 	7427.72	(0.02)	45(14,31) - 45(14,32)		[72069]
	7439.68	(0.02)	68(21,47) - 68(21,48)		[72069]
	7466.79	(0.03)	29(9,20) - 29(9,21)	2ν ₂₃	[72069]
	7544.63	(0.02)	29(9,20) - 29(9,21)	1ν 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	[72069]
	7657.98	(0.03)	29(9,20) - 29(9,21)	1ν ₂₃ 1ν ₄₈	[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 ₂₃	[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	2v c	[76061]
	19730.04	(0.03)	6 - 5	1v c	[76061]
	19731.73	(0.03)	6 - 5		[76061]
	19737.96	(0.03)	6 - 5	1v a	[76061]
	19739.73	(0.03)	6 - 5	1v b	[76061]
	19744.03	(0.03)	6 - 5	2v a	[76061]
	19745.87	(0.03)	6 - 5	1v a	1v b [76061]
	19747.64	(0.03)	6 - 5	2v b	[76061]
	23016.53	(0.03)	7 - 6	2v c	[76061]
	23018.37	(0.03)	7 - 6	1v c	[76061]
	23020.33	(0.03)	7 - 6		[76061]
	23027.58	(0.03)	7 - 6	1v a	[76061]
	23029.65	(0.03)	7 - 6	1v b	[76061]
	23034.68	(0.03)	7 - 6	2v a	[76061]
	23036.83	(0.03)	7 - 6	1v a	1v b [76061]
	23038.92	(0.03)	7 - 6	2v b	[76061]
	23052.99	(0.03)	7 - 6	2v a	2v b [76061]
	26304.54	(0.03)	8 - 7	2v c	[76061]
	26306.67	(0.03)	8 - 7	1v c	[76061]
	26308.92	(0.03)	8 - 7		[76061]
	26317.20	(0.03)	8 - 7	1v a	[76061]
	26319.58	(0.03)	8 - 7	1v b	[76061]
	26325.30	(0.03)	8 - 7	2v a	[76061]
	26327.77	(0.03)	8 - 7	1v a	1v b [76061]
	26330.17	(0.03)	8 - 7	2v b	[76061]
	26346.21	(0.03)	8 - 7	2v a	2v b [76061]
	29592.49	(0.03)	9 - 8	2v c	[76061]
	29594.91	(0.03)	9 - 8	1v c	[76061]
	29597.48	(0.01)	9 - 8		[75059]
	29603.96	(0.03)	9 - 8	1v a	1v c [76061]
	29605.65	(0.03)	9 - 8	1v d	[76061]
	29606.82	(0.03)	9 - 8	1v a	[76061]
	29609.47	(0.03)	9 - 8	1v b	[76061]
	29612.62	(0.03)	9 - 8	1v e	[76061]
	29615.92	(0.03)	9 - 8	2v a	[76061]
	29618.75	(0.03)	9 - 8	1v a	1v b [76061]
	29621.32	(0.03)	9 - 8	2v b	[76061]
	29625.10	(0.03)	9 - 8	3v a	[76061]
	29627.65	(0.03)	9 - 8	2v a	1v b [76061]
	32880.60	(0.03)	9 - 8	2v c	[76061]
	32883.25	(0.03)	9 - 8	1v c	[76061]
	32885.99	(0.01)	10 - 9		[75059]
	32890.82	(0.03)	10 - 9	1v a	$\ell = l_1$ [76061]
	32893.24	(0.03)	10 - 9	1v a	1v c [76061]
	32895.06	(0.03)	10 - 9	1v d	[76061]
	32896.38	(0.03)	10 - 9	1v a	[76061]
	32899.36	(0.03)	10 - 9	1v b	[76061]
	32901.98	(0.03)	10 - 9	1v a	$\ell = u_1$ [76061]
	32902.87	(0.03)	10 - 9	1v e	[76061]
32906.51	(0.03)	10 - 9	2v a	[76061]	
32908.35	(0.03)	10 - 9	1v b	1v d [76061]	
32909.62	(0.03)	10 - 9	1v a	1v b [76061]	
32912.65	(0.03)	10 - 9	2v b	[76061]	
32916.50	(0.03)	10 - 9	3v a	[76061]	
32919.65	(0.03)	10 - 9	2v a	1v b [76061]	
32922.80	(0.03)	10 - 9	1v a	2v b [76061]	
32926.00	(0.03)	10 - 9	3v b	[76061]	
36168.60	(0.03)	11 - 10	2v c	[76061]	
36171.45	(0.03)	11 - 10	1v c	[76061]	
36174.55	(0.01)	11 - 10		[75059]	
36179.76	(0.03)	11 - 10	1v a	$\ell = l_1$ [76061]	
36182.50	(0.03)	11 - 10	1v a	1v c [76061]	
36184.70	(0.03)	11 - 10	1v d	[76061]	
36185.95	(0.03)	11 - 10	1v a	[76061]	
36189.24	(0.03)	11 - 10	1v b	[76061]	
36192.00	(0.03)	11 - 10	1v a	$\ell = u_1$ [76061]	
36193.06	(0.03)	11 - 10	1v 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	2ν a	[76061]
	36199.28	(0.03)	11 - 10	1ν b	[76061]
	36200.42	(0.03)	11 - 10	1ν a	[76061]
	36203.72	(0.03)	11 - 10	2ν b	[76061]
	36208.02	(0.03)	11 - 10	3ν a	[76061]
	36211.52	(0.03)	11 - 10	2ν a	[76061]
	36214.88	(0.03)	11 - 10	1ν a	[76061]
	36225.92	(0.03)	11 - 10	2ν a	[76061]
	39456.51	(0.01)	12 - 11	2ν c	[76061]
	39459.69	(0.01)	12 - 11	1ν c	[76061]
	39463.05	(0.01)	12 - 11		[75059]
	39468.74	(0.03)	12 - 11	1ν a	[76061]
	39471.83	(0.01)	12 - 11	1ν a	[76061]
	39473.93	(0.01)	12 - 11	1ν d	[76061]
	39475.48	(0.01)	12 - 11	1ν a	[76061]
	39479.06	(0.01)	12 - 11	1ν b	[76061]
	39482.10	(0.01)	12 - 11	1ν a	[76061]
	39483.32	(0.01)	12 - 11	1ν e	[76061]
	39487.68	(0.01)	12 - 11	2ν a	[76061]
	39490.00	(0.01)	12 - 11	1ν b	[76061]
	39491.35	(0.01)	12 - 11	1ν a	[76061]
	39494.94	(0.01)	12 - 11	2ν b	[76061]
	39499.60	(0.01)	12 - 11	3ν a	[76061]
	39503.38	(0.01)	12 - 11	2ν a	[76061]
	39507.12	(0.01)	12 - 11	1ν a	[76061]
	39510.70	(0.01)	12 - 11	3ν b	[76061]
	39519.01	(0.01)	12 - 11	2ν a	[76061]

3. References to Spectral Data

- [50022] R. Trambarulo and W. Gordy, *J. Chem. Phys.* **18**, 1613 (1950).
- [55018] L. F. Thomas, E. I. Sherrard, and J. Sheridan, *Trans. Faraday Soc.* **51**, 619 (1955).
- [55019] G. A. Heath, L. F. Thomas, E. I. Sherrard, and J. Sheridan, *Faraday Soc. Discussions* **19**, 38 (1955).
- [56018] V. W. Laurie, *J. Chem. Phys.* **24**, 635L (1956).
- [57014] C. A. Burrus and W. Gordy, *J. Chem. Phys.* **26**, 391 (1957).
- [57015] D. R. Lide, Jr. and D. E. Mann, *J. Chem. Phys.* **27**, 868 (1957).
- [57016] D. R. Lide, Jr. and D. E. Mann, *J. Chem. Phys.* **27**, 874 (1957).
- [57017] L. F. Thomas, J. S. Heeks, and J. Sheridan, *Archives des Sci.* **10**, 180 (1957).
- [58009] D. R. Herschbach and L. C. Krisher, *J. Chem. Phys.* **28**, 728 (1958).
- [58010] D. R. Lide, Jr. and D. E. Mann, *J. Chem. Phys.* **29**, 914 (1958).
- [59017] P. H. Kasai, R. J. Myers, D. F. Eggers, Jr., and K. B. Wiberg, *J. Chem. Phys.* **30**, 512 (1959).
- [60008] V. W. Zeil, M. Winnewisser, H. K. Bodensch, and H. Buchert, *Z. Naturforsch.* **15a**, 1011 (1960).
- [60009] D. R. Lide, Jr., *J. Chem. Phys.* **33**, 1514 (1960).
- [60010] D. R. Lide, Jr., *J. Chem. Phys.* **33**, 1519 (1960).
- [61013] D. R. Lide, Jr. and D. Christensen, *J. Chem. Phys.* **35**, 1374 (1961).
- [61014] V. W. Laurie, *J. Chem. Phys.* **34**, 1516 (1961).
- [62022] L. J. Nugent, D. E. Mann, and D. R. Lide, Jr., *J. Chem. Phys.* **36**, 965 (1962).
- [62023] G. W. Rathjens, *J. Chem. Phys.* **36**, 2401 (1962).
- [62027] L. H. Scharpen and V. W. Laurie, *J. Chem. Phys.* **39**, 1732 (1963).
- [64028] D. R. Lide, Jr. and M. Jen, *J. Chem. Phys.* **40**, 252 (1964).
- [64029] J. S. Muentner and V. W. Laurie, *J. Am. Chem. Soc.* **86**, 3901 (1964).
- [65029] H. Kim and W. D. Gwinn, *J. Chem. Phys.* **42**, 3728 (1965).
- [65030] L. H. Scharpen and V. W. Laurie, *J. Chem. Phys.* **43**, 2765 (1965).
- [65031] S. S. Butcher, *J. Chem. Phys.* **42**, 1830 (1965).
- [65032] G. Luss and M. D. Harmony, *J. Chem. Phys.* **43**, 3768 (1965).
- [65033] S. S. Butcher, *J. Chem. Phys.* **42**, 1833 (1965).
- [65034] H. J. Tobler, A. Bauder, and Hs. H. Günthard, *J. Mol. Spectrosc.* **18**, 239 (1965).
- [65035] S. S. Butcher and C. C. Costain, *J. Mol. Spectrosc.* **15**, 40 (1965).
- [66041] M. D. Harmony and K. Cox, *J. Am. Chem. Soc.* **88**, 5049 (1966).
- [66042] J. S. Muentner and V. W. Laurie, *J. Chem. Phys.* **45**, 855 (1966).
- [66043] V. W. Weiss and W. H. Flygare, *J. Chem. Phys.* **45**, 8 (1966).
- [66044] E. Hirota and Y. Morino, *J. Chem. Phys.* **45**, 2326 (1966).
- [66045] E. Hirota, *J. Chem. Phys.* **45**, 1984 (1966).
- [67033] E. Hirota, C. Matsumura and Y. Morino, *Bull. Chem. Soc. Japan* **40**, 1124 (1967).
- [67034] H. D. Rudolph, H. Dreizler, A. Jaeschke, and P. Wendling, *Z. Naturforsch.* **22a**, 940 (1967).
- [68043] S. Kondo, E. Hirota, and Y. Morino, *J. Mol. Spectrosc.* **28**, 471 (1968).
- [68044] L. H. Scharpen and V. W. Laurie, *J. Chem. Phys.* **49**, 3041 (1968).
- [68046] L. H. Scharpen, J. E. Wollrab, and D. P. Ames, *J. Chem. Phys.* **49**, 2368 (1968).
- [68047] E. Hirota, T. Hirooka, and Y. Morino, *J. Mol. Spectrosc.* **26**, 351 (1968).
- [68048] R. G. Ford and R. A. Beaudet, *J. Chem. Phys.* **48**, 4671 (1968).
- [68049] T. N. Sarachman, *J. Chem. Phys.* **49**, 3146 (1968).
- [69055] R. C. Benson and W. H. Flygare, *J. Chem. Phys.* **51**, 3087 (1969).
- [69056] B. Bak, J. J. Led, L. Nygaard, J. Rastrup-Andersen, and G. O. Sorensen, *J. Mol. Struct.* **3**, 369 (1969).
- [69057] K. Cox, M. D. Harmony, G. Nelson, and K. B. Wiberg, *J. Chem. Phys.* **50**, 1976 (1969).
- [69058] S. L. Hsu, M. K. Kemp, J. M. Pochan, R. C. Benson, and W. H. Flygare, *J. Chem. Phys.* **50**, 1482 (1969).
- [69060] J. M. Pochan and W. H. Flygare, *J. Am. Chem. Soc.* **91**, 5928 (1969).
- [69061] T. Ogata and K. Kozima, *Bull. Chem. Soc. Japan* **42**, 1263 (1969).
- [69062] J. S. McKnight and W. Gordy, *Bull. Am. Phys. Soc.* **14**, 621 (1969).
- [69063] A. Bauer and J. Burie, *C. R. Acad. Sci. (Paris)* **268B**, 800 (1969).
- [69064] R. L. Shoemaker and W. H. Flygare, *J. Am. Chem. Soc.* **91**, 5417 (1969).
- [69065] R. C. Benson and W. H. Flygare, *Chem. Phys. Lett.* **4**, 141 (1969).
- [69066] M. K. Kemp and W. H. Flygare, *J. Am. Chem. Soc.* **91**, 3163 (1969).
- [69067] S. L. Hsu and W. H. Flygare, *J. Mol. Spectrosc.* **32**, 375 (1969).
- [70029] L. H. Scharpen, J. S. Muentner, and V. W. Laurie, *J. Chem. Phys.* **53**, 2513 (1970).
- [70061] C. Hirose, *Bull. Chem. Soc. Japan* **43**, 3695 (1970).
- [70062] V. W. Laurie and W. M. Stigliani, *J. Am. Chem. Soc.* **92**, 1485 (1970).
- [70063] R. C. Benson and W. H. Flygare, *J. Chem. Phys.* **53**, 4470 (1970).
- [70064] S. L. Hsu, A. H. Andrist, T. D. Gierke, R. C. Benson, W. H. Flygare, and J. E. Baldwin, *J. Am. Chem. Soc.* **92**, 5250 (1970).
- [70065] R. C. Benson and W. H. Flygare, *J. Am. Chem. Soc.* **92**, 7523 (1970).
- [70066] E. Hirota, *J. Mol. Spectrosc.* **34**, 516 (1970).
- [70067] S. Kondo, Y. Sakurai, E. Hirota, and Y. Morino, *J. Mol. Spectrosc.* **34**, 231 (1970).
- [70068] S. C. Wofsy, J. S. Muentner, and W. Klemperer, *J. Chem. Phys.* **53**, 4005 (1970).
- [70069] Y. S. Huang and R. A. Beaudet, *J. Chem. Phys.* **52**, 935 (1970).
- [70070] S. L. Hsu and W. H. Flygare, *J. Chem. Phys.* **52**, 1053 (1970).
- [71045] T. D. Gierke, S. L. Hsu, and W. H. Flygare, *J. Mol. Spectrosc.* **40**, 328 (1971).
- [71046] D. Damiani and A. M. Mirri, *Chem. Phys. Lett.* **10**, 351 (1971).
- [71047] E. Hirota and C. Matsumura, *J. Chem. Phys.* **55**, 981 (1971).
- [71048] I. Ozier, *Phys. Rev. Letters* **27**, 1329 (1971).
- [71049] R. G. Ford and R. A. Beaudet, *J. Chem. Phys.* **55**, 3110 (1971).
- [71050] J. Demaison and H. D. Rudolph, *J. Mol. Spectrosc.* **40**, 445 (1971).
- [72061] T. D. Gierke, R. C. Benson, and W. H. Flygare, *J. Am. Chem. Soc.* **94**, 339 (1972).
- [72062] M. J. Collins, C. O. Britt, and J. E. Boggs, *J. Chem. Phys.* **56**, 4262 (1972).
- [72063] F. J. Wodarczyk and E. B. Wilson, *J. Chem. Phys.* **56**, 166 (1972).
- [72064] R. D. Suenram and M. D. Harmony, *J. Chem. Phys.* **56**, 3837 (1972).
- [72065] R. D. Suenram and M. D. Harmony, *J. Am. Chem. Soc.* **94**, 5915 (1972).

- [72066] P. A. Baron, R. D. Brown, F. R. Burden, P. J. Domaille, and J. E. Kent, *J. Mol. Spectrosc.* **43**, 401 (1972).
- [72067] R. D. Suenram and M. D. Harmony, unpublished data (1972).
- [72068] J. R. Durig, Y. S. Li, and L. A. Carreira, *J. Chem. Phys.* **57**, 1896 (1972).
- [72069] P. Christen, A. Bauder, and Hs. H. Günthard, *J. Mol. Spectrosc.* **43**, 1 (1972).
- [72070] R. D. Suenram and M. D. Harmony, *J. Chem. Phys.* **57**, 2597 (1972).
- [73076] R. D. Suenram and M. D. Harmony, *J. Am. Chem. Soc.* **95**, 4506 (1973).
- [73077] R. D. Suenram and M. D. Harmony, *J. Chem. Phys.* **58**, 5842L (1973).
- [73079] A. R. Mochel, A. Bjorseth, C. O. Britt, and J. E. Boggs, *J. Mol. Spectrosc.* **48**, 107 (1973).
- [73080] J. L. Duncan, D. C. McKean, P. D. Mallinson, and R. D. McCulloch, *J. Mol. Spectrosc.* **46**, 232 (1973).
- [73081] E. Hirota and C. Matsumura, *J. Chem. Phys.* **59**, 3038 (1973).
- [73082] R. F. Curl, Jr., *J. Mol. Spectrosc.* **48**, 165 (1973).
- [73083] M. Takami, K. Uchara, and K. Shimoda, *Jpn. J. Appl. Phys.* **12**, 924 (1973).
- [73084] A. Trinkaus, H. Dreizler, and H. D. Rudolph, *Z. Naturforsch.* **82a**, 750 (1973).
- [73085] W. A. Kreiner, H. D. Rudolph, and B. T. Tan, *J. Mol. Spectrosc.* **48**, 86 (1973).
- [73086] H. D. Rudolph, K. Walzer, and I. Krutzik, *J. Mol. Spectrosc.* **47**, 314 (1973).
- [74055] O. E. H. Rydbeck, J. Eilddér, W. M. Irvine, A. Sume and Å. Hjalmarson, *Astron. Astrophys.* **34**, 479 (1974).
- [74063] F. G. Codding and R. H. Schwendeman, *J. Mol. Spectrosc.* **49**, 226 (1974).
- [74064] D. W. T. Griffith and J. E. Kent, *Chem. Phys. Lett.* **25**, 290 (1974).
- [74065] R. L. Cook, T. B. Malloy, *J. Am. Chem. Soc.* **96**, 1703 (1974).
- [75050] W. M. Stigliani, V. W. Laurie, and J. C. Li, *J. Chem. Phys.* **62**, 1890 (1975).
- [75051] R. D. Suenram, *J. Am. Chem. Soc.* **97**, 4869 (1975).
- [75052] T. K. Avirah, R. L. Cook, and T. B. Malloy, Jr., *J. Mol. Spectrosc.* **54**, 231 (1975).
- [75053] M. D. Harmony, C. S. Wang, K. B. Wiberg, and K. C. Bishop, III, *J. Chem. Phys.* **63**, 3312 (1975).
- [75054] A. P. Cox, I. C. Ewart, and W. M. Stigliani, *J. Chem. Soc. Faraday Trans. 7*, 504 (1975).
- [75055] L. Engelbrecht and D. H. Sutter, *Z. Naturforsch.* **30a**, 1265 (1975).
- [75056] C. W. Holt, M. C. L. Gerry, and I. Ozier, *Can. J. Phys.* **53**, 1791 (1975).
- [75057] E. Hirota and M. Imachi, *Can. J. Phys.* **53**, 2023 (1975).
- [75058] J. Demaison and H. D. Rudolph, *J. Mol. Struct.* **24**, 325 (1975).
- [75059] E. A. C. Lucken, R. Pozzi, and K. R. Ramaprasad, *J. Mol. Struct.* **26**, 259 (1975).
- [76052] S. N. Mathur, M. D. Harmony, and R. D. Suenram, *J. Chem. Phys.* **64**, 4340 (1976).
- [76054] C. S. Wang and M. D. Harmony, *J. Am. Chem. Soc.* **98**, 1108 (1976).
- [76055] A. Bauder, C. Keller, and M. Neuenschwander, *J. Mol. Spectrosc.* **63**, 281 (1976).
- [76058] J. L. Duncan, *J. Mol. Spectrosc.* **60**, 225 (1976).
- [76059] I. Ozier, R. M. Lees, and M. C. L. Gerry, *J. Chem. Phys.* **65**, 1795 (1976).
- [76060] J. Demaison, D. Schwach, B. T. Tan, and H. D. Rudolph, *J. Mol. Spectrosc.* **60**, 324 (1976).
- [76061] W. M. Stigliani and V. W. Laurie, *J. Mol. Spectrosc.* **60**, 188 (1976).
- [77036] R. D. Suenram and F. J. Lovas, unpublished data (1977).
- [77037] J. F. Chiang, R. Chaing, K. C. Lu, E. M. Sung, and M. D. Harmony, *J. Mol. Struct.* **41**, 61 (1977).
- [77038] W. J. Lafferty, R. D. Suenram, and D. R. Johnson, *J. Mol. Spectrosc.* **64**, 147 (1977).
- [77039] E. Hirota, K. Matsumura, M. Imachi, M. Fujio, Y. Tsuno and C. Matsumura, *J. Chem. Phys.* **66**, 2660 (1977).
- [77040] J. Demaison, D. Schwach, B. T. Tan, and H. D. Rudolph, *J. Mol. Spectrosc.* **68**, 97 (1977).
- [78029] K. B. Wiberg, G. B. Ellison, J. J. Wendolosky, W. E. Pratt, and M. D. Harmony, *J. Am. Chem. Soc.* **100**, 7837 (1978).
- [78030] S. N. Mathur and M. D. Harmony, *J. Mol. Spectrosc.* **69**, 37 (1978).
- [78031] A. Dubrulle, D. Boucher, J. Burie, and J. Demaison, *J. Mol. Spectrosc.* **72**, 158 (1978).
- [78032] M. G. Guélin, S. Green, and P. Thaddeus, *Astrophys. J.* **224**, L27 (1978).
- [78033] I. Ozier and A. Rosenberg, *J. Chem. Phys.* **69**, 5203 (1978).
- [78034] A. J. Alexander, H. W. Kroto, M. Maier, and D. R. M. Walton, *J. Mol. Spectrosc.* **70**, 84 (1978).
- [79031] S. N. Mathur and M. D. Harmony, *J. Mol. Struct.* **57**, 63 (1979).
- [79032] R. A. Creswell, M. Pagitsas, P. Shoja-Chaghervand, and R. H. Schwendeman, *J. Phys. Chem.* **83**, 1427 (1979).
- [79033] A. Bouchy, G. Roussy, M. J. Ledoux, and F. G. Gault, *J. de Chim. Physique* **76**, 357 (1979).
- [79034] T. K. Avirah, T. B. Malloy, Jr., and R. L. Cook, *J. Chem. Phys.* **71**, 2194 (1979).
- [79035] T. K. Avirah, R. L. Cook, and T. B. Malloy, Jr., *J. Chem. Phys.* **71**, 3478 (1979).
- [79036] Y. S. Li, M. R. Jalilian, and J. R. Durig, *J. Mol. Spectrosc.* **51**, 171 (1979).
- [79037] E. Hirota, S. Saito, and Y. Endo, *J. Chem. Phys.* **71**, 1183 (1979).
- [79038] A. Bauer, D. Boucher, J. Burie, J. Demaison, and A. Dubrulle, *J. Phys. Chem. Ref. Data* **8**, 537 (1979).
- [79039] P. Guyon, A. Bouchy, and G. Roussy, *J. Mol. Struct.* **57**, 53 (1979).
- [80032] E. Torneng, C. J. Nielsen, P. Klæboe, H. Hopf, and H. Priebe, *Spectrochim. Acta* **36A**, 975 (1980).
- [80033] A. Bouchy and M. J. Ledoux, *J. Mol. Spectrosc.* **80**, 453 (1980).
- [80034] A. Choplin, *Chem. Phys. Lett.* **71**, 503 (1980).
- [80035] S. W. Staley, A. E. Howard, M. D. Harmony, S. N. Mathur, M. K. Ari, J. I. Choe, and G. Lind, *J. Am. Chem. Soc.* **102**, 3639 (1980).
- [80036] D. Damiani, G. Corbelli, and F. Scappini, *J. Mol. Struct.* **63**, 221 (1980).
- [80037] K. Matsumura, T. Tanaka, Y. Endo, S. Saito, and E. Hirota, *J. Phys. Chem.* **84**, 1793 (1980).
- [80038] P. M. Burrell, E. Bjarnov, and R. H. Schwendeman, *J. Mol. Spectrosc.* **82**, 193 (1980).
- [80039] H. M. Pickett, E. A. Cohen, and T. G. Phillips, *Astrophys. J. (Letters)* **236**, L43 (1980).
- [80040] W. M. Itano and I. Ozier, *J. Chem. Phys.* **72**, 3700 (1980).
- [81036] R. L. Kuczkowski, F. J. Lovas, R. D. Suenram, R. P. Latimer, K. W. Hillig, II, and A. J. Ashe, III, *J. Mol. Struct.* **72**, 143 (1981).
- [81037] B. P. van Eijck, *J. Mol. Spectrosc.* **85**, 189 (1981).
- [81038] A. Bouchy and G. Roussy, *J. de Chim. Physique* **78**, 669 (1981).
- [81040] M. D. Harmony, S. N. Mathur, J. I. Choe, M. K. Ari, A. E. Howard, and S. W. Staley, *J. Am. Chem. Soc.* **103**, 2961 (1981).
- [81042] E. Hirota, Y. Endo, S. Saito, and K. Yoshida, *J. Mol. Spectrosc.* **89**, 223 (1981).
- [81043] E. Hirota, Y. Endo, S. Saito, and J. L. Duncan, *J. Mol. Spectrosc.* **89**, 285 (1981).
- [81044] I. Ozier, M. C. L. Gerry, and A. G. Robiette, *J. Phys. Chem. Ref. Data* **10**, 1085 (1981).
- [81045] W. A. Kreiner and A. G. Robiette, *J. Chem. Phys.* **74**, 3713 (1981).
- [81046] K. Matsumura, T. Etoh, and T. Tanaka, *J. Mol. Spectrosc.* **90**, 106 (1981).

- [81047] I. Etoh, K. Matsumura, and T. Tanaka, *J. Mol. Spectrosc.* **89**, 511 (1981).
- [81048] V. Amir-Ebrahimi, A. Choplin, J. Demaison, and G. Roussy, *J. Mol. Spectrosc.* **89**, 42 (1981).
- [82032] Per Jensen, P. R. Bunker, and A. R. Hoy, *J. Chem. Phys.* **77**, 5370 (1982).
- [82033] T. J. Sears, P. R. Bunker, and A. R. W. McKellar, *J. Chem. Phys.* **77**, 5363 (1982).
- [82034] T. J. Sears, P. R. Bunker, A. R. W. McKellar, K. M. Evenson, D. A. Jennings, and J. M. Brown, *J. Chem. Phys.* **77**, 5348 (1982).
- [82035] C. D. Cogley, L. M. Tack, and S. G. Kukolich, *J. Chem. Phys.* **76**, 5669 (1982).
- [82036] K. Matsumura and T. Tanaka, *J. Mol. Spectrosc.* **96**, 219 (1982).
- [83012] C. R. Brazier and J. M. Brown, *J. Chem. Phys.* **78**, 1608 (1983).
- [83028] M. Bogey, C. Demuynck, and J. L. Destombes, *Chem. Phys. Lett.* **100**, 105 (1983).
- [83033] R. D. Brown, P. D. Godfrey, B. T. Hart, A. H. O'trey, M. Onda and M. Woodruff, *Aust. J. Chem.* **36**, 639 (1983).
- [83034] R. N. Nandi and M. D. Harmony, *J. Mol. Spectrosc.* **98**, 221 (1983).
- [83038] B. M. Landsberg and R. D. Suenram, *J. Mol. Spectrosc.* **98**, 210 (1983).
- [83039] J. Demaison, D. Boucher, J. Burie, and A. Dubrulle, *Z. Naturforsch.* **38a**, 447 (1983).
- [83046] F. J. Lovas, R. D. Suenram, and K. M. Evenson, *Astrophys. J.* **267**, L131 (1983).
- [83048] P. R. Bunker and Per Jensen, *J. Chem. Phys.* **79**, 1224 (1983).
- [83049] A. R. W. McKellar and T. J. Sears, *Can. J. Phys.* **61**, 480 (1983).
- [83050] P. R. Bunker, T. J. Sears, A. R. W. McKellar, K. M. Evenson, and F. J. Lovas, *J. Chem. Phys.* **79**, 1211 (1983).
- [83051] M. D. Harmony, R. N. Nandi, J. V. Tietz, J. -I. Choe, S. J. Getty, and S. W. Staley, *J. Am. Chem. Soc.* **105**, 3947 (1983).
- [83052] M. B. Bell, H. E. Matthews, and T. J. Sears, *Astron. Astrophys.* **127**, 241 (1983).
- [83053] C. A. Gottlieb, E. W. Gottlieb, P. Thaddeus, and H. Kawamura, *Astrophys. J.* **275**, 916 (1983).
- [83054] W. A. Kreiner and R. Opferkuch, *J. Mol. Struct.* **97**, 289 (1983).
- [83055] A. R. W. McKellar, C. Yamada, and E. Hirota, *J. Chem. Phys.* **79**, 1220 (1983).
- [83059] R. N. Nandi, M. D. Harmony, A. E. Howard, and S. W. Staley, *J. Chem. Phys.* **78**, 3560 (1983).
- [84026] Y. S. Li, *J. Phys. Chem.* **88**, 4049 (1984).
- [84027] J. Nakagawa, M. Hayashi, Y. Endo, S. Saito, and E. Hirota, *J. Chem. Phys.* **80**, 5922 (1984).
- [84028] K. M. Evenson, T. J. Sears, and A. R. W. McKellar, *J. Opt. Soc. Am. B* **1**, 15 (1984).
- [84029] W. Hüttner, H. Häussler, and W. Majer, *Chem. Phys. Lett.* **109**, 359 (1984).
- [84030] I. Ozier and W. L. Meerts, *Can. J. Phys.* **62**, 1844 (1984).
- [84031] M. Oldani and A. Bauder, *Chem. Phys. Lett.* **108**, 7 (1984).
- [84032] J. M. Ware and J. A. Roberts, *J. Chem. Phys.* **81**, 1215 (1984).
- [84033] C. R. Brazier and J. M. Brown, *Can. J. Phys.* **62**, 1563 (1984).
- [84034] H. Suzuki, N. Kaifu, J. Miyaji, M. Morimoto, M. Ohishi, and S. Saito, private communication, (1984).
- [84035] M. Bester, K. Yamada, G. Winnewisser, W. Joentgen, H. J. Altenbach, E. Vogel, *Astron. Astrophys. (Letters)* **137**, L20 (1984).
- [84036] C. M. Walmsley, P. R. Jewell, L. E. Snyder, and G. Winnewisser, *Astron. Astrophys. (Letters)* **134**, L11 (1984).
- [84037] K. Matsumura and T. Tanaka, *J. Mol. Spectrosc.* **108**, 299 (1984).
- [85000] M. Bogey, C. Demuynck, and J. L. Destombes, *Astron. Astrophys.* **144**, L15 (1985).
- [85006] C. A. Gottlieb, J. M. Vrtilik, E. W. Gottlieb, and P. Thaddeus, *Astrophys. J. (Letters)* **294**, L55 (1985).
- [85007] J. M. Vrtilik, C. A. Gottlieb, W. D. Langer, P. Thaddeus, and R. W. Wilson, *Astrophys. J. (Letters)* **296**, L35 (1985).
- [85014] G. Bestmann and H. Dreizler, *Z. Naturforsch.* **40a**, 263 (1985).
- [85015] J. M. Ware, J. A. Roberts, *J. Chem. Phys.* **82**, 5 (1985).
- [85016] L. M. Ziurys and B. E. Turner, *Astrophys. J. (Letters)* **292**, L25 (1985).
- [85017] T. C. Steimle, D. R. Woodward, and J. M. Brown, *Astrophys. J. (Letters)* **294**, L59 (1985).
- [85018] H. E. Matthews and W. Irvine, *Astrophys. J. (Letters)* **298**, L61 (1985).
- [85019] P. Thaddeus, J. M. Vrtilik, and C. A. Gottlieb, *Astrophys. J. (Letters)* **299**, L63 (1985).
- [85020] M. Oldani, M. Andrist, A. Bauder, and A. G. Robiette, *J. Mol. Spectrosc.* **110**, 93 (1985).
- [85021] M. Oldani, A. Bauder, M. Locta, J. P. Champion, G. Pierre, J. C. Hilico, and A. G. Robiette, *J. Mol. Spectrosc.* **113**, 229 (1985).
- [85022] G. Bestmann, H. Dreizler, J. M. Vacherand, D. Boucher, B. P. van Eijck, and J. Demaison, *Z. Naturforsch.* **40a**, 508 (1985).
- [85023] G. Bestmann, W. Lalowski, and H. Dreizler, *Z. Naturforsch.* **40a**, 271 (1985).
- [86004] C. A. Gottlieb, E. W. Gottlieb, and P. Thaddeus, *Astron. Astrophys. (Letters)* **164**, L5 (1986).
- [86005] R. D. Brown, P. D. Godfrey, and M. Rodler, *J. Am. Chem. Soc.* **108**, 1296 (1986).
- [86006] M. Bogey, C. Demuynck, J. L. Destombes, and J. C. Guillemin, *Chem. Phys. Lett.* **125**, 569 (1986).
- [86007] V. Prakash and J. A. Roberts, *J. Chem. Phys.* **84**, 1193 (1986).
- [86008] M. Bogey, C. Demuynck, and J. L. Destombes, *Chem. Phys. Lett.* **125**, 383 (1986).
- [86009] M. Bogey and J. L. Destombes, *Astron. Astrophys. (Letters)* **159**, L8 (1986).
- [86010] C. A. Gottlieb, E. W. Gottlieb, P. Thaddeus, and J. M. Vrtilik, *Astrophys. J.* **303**, 446 (1986).
- [86011] R. Widmer, M. Oldani, and A. Bauder, *J. Mol. Spectrosc.* **116**, 259 (1986).
- [86012] B. Vogelsanger, M. Oldani, and A. Bauder, *J. Mol. Spectrosc.* **119**, 214 (1986).
- [86013] T. D. Norden, S. T. Staley, W. H. Taylor, and M. D. Harmony, *J. Am. Chem. Soc.* **108**, 7912 (1986).
- [86018] T. C. Steimle, D. R. Woodward, and J. M. Brown, *J. Chem. Phys.* **85**, 1276 (1986).
- [86019] W. M. Rhee and J. A. Roberts, *J. Chem. Phys.* **85**, 6940 (1986).
- [86020] W. M. Rhee, J. A. Roberts, and V. Prakash, *J. Mol. Spectrosc.* **120**, 169 (1986).
- [86021] J. M. Ware, V. Prakash, and J. A. Roberts, *J. Mol. Spectrosc.* **116**, 17 (1986).
- [86022] H. Suzuki, M. Ohishi, N. Kaifu, S. -I. Ishikawa, T. Kasuga, S. Saito, and K. Kawaguchi, *Publ. Astron. Soc. Japan* **38**, 911 (1986).
- [86024] J. Cernicharo, C. Kahane, J. Gomez-Gonzalez, and M. Guélin, *Astron. Astrophys.* **164**, L1 (1986).
- [87002] E. Fliege and H. Dreizler, *Z. Naturforsch.* **42a**, 72 (1987).
- [87003] W. A. Kreiner, P. Müller, L. Jörissen, M. Oldani, and A. Bauder, *Can. J. Phys.* **65**, 32 (1987).

- [87004] M. Bogey, C. Demuyneck, J. L. Destombes, and H. Dubus, *J. Mol. Spectrosc.* **122**, 313 (1987).
- [87005] S. Yamamoto, S. Saito, M. Ohishi, H. Suzuki, S. -I. Ishikawa, N. Kaifu, and A. Murakami, *Astrophys. J. (Letters)*, **332**, L55 (1987).
- [87006] S. Saito, K. Kawaguchi, H. Suzuki, M. Ohishi, N. Kaifu, and S. -I. Ishikawa, *Publ. Astron. Soc. Japan* **39**, 193 (1987).
- [87007] M. Guélin, J. Cernicharo, C. Kahane, J. Gomez-Gonzales, and C. M. Walmsley, *Astron. Astrophys.* **175**, L5 (1987).
- [87008] J. M. Vrtilik, C. A. Gottlieb, T. J. LePage, and P. Thaddeus, *Astrophys. J.* **316**, 826 (1987).
- [87009] J. Cernicharo, M. Guélin, K. M. Menten, and G. M. Walmsley, *Astron. Astrophys.* **181**, L1 (1987).
- [87011] R. D. Brown, P. D. Godfrey, and R. P. A. Bettens, *Mon. Not. R. Astron. Soc.* **227**, 19p (1987).
- [87012] J. Cernicharo, M. Guélin, and C. M. Walmsley, *Astron. Astrophys.* **172**, L5 (1987).
- [87013] M. Oldani, A. Bauder, J. C Hilico, M. Lorte, and J. P. Champion, *Europhys. Lett.* **4**, 29 (1987).
- [87016] M. B. Bell, J. K. G. Watson, P. A. Feldman, H. E. Matthews, S. C. Madden, and W. M. Irvine, *Chem. Phys. Lett.* **136**, 588 (1987).
- [87017] B. Vogelsanger and A. Bauder, *J. Chem. Phys.* **87**, 4465 (1987).
- [87018] M. Guélin, J. Cernicharo, S. Navarro, D. R. Woodward, C. A. Gottlieb, and P. Thaddeus, *Astron. Astrophys.* **182**, L37 (1987).
- [87019] Y. Endo, M. C. Chang, and E. Hirota, *J. Mol. Spectrosc.* **126**, 63 (1987).
- [87020] D. R. Woodward, J. C. Pearson, C. A. Gottlieb, M. Guélin, and P. Thaddeus, *Astron. Astrophys.* **186**, L14 (1987).
- [87021] T. Ogata, A. Mochizuki, and E. Yamashita, *J. Chem. Phys.* **87**, 2531 (1987).
- [87022] H. Kanata, S. Yamamoto, and S. Saito, *Chem. Phys. Lett.* **140**, 221 (1987).
- [87023] R. L. DeLeon and J. S. Muentzer, *J. Mol. Spectrosc.* **126**, 13 (1987).
- [87024] B. Vogelsanger, W. Caminati, and A. Bauder, *Chem. Phys. Lett.* **141**, 245 (1987).
- [87027] D. R. Woodward, J. C. Pearson, C. A. Gottlieb, M. Guélin, and P. Thaddeus, *Astron. Astrophys.* **186**, L14 (1987).
- [88001] J. C. Pearson, C. A. Gottlieb, D. R. Woodward, and P. Thaddeus, *Astron. Astrophys.* **189**, L13 (1988).