Microwave Study and Molecular Structure of Fluorinated Benzonitriles

By

Mahdi Kamaee

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Abstract

In this thesis work, the results of microwave investigation and structural determination for benzonitrile and some of its fluorinated derivatives are presented. Two custom-built Fourier transform microwave (FTMW) spectrometers at the University of Manitoba including the Balle-Flygare FTMW and Chirped pulse-FTMW instruments were used to record the pure rotational spectra of the studied compounds including benzonitrile, 2-fluorobenzonitrile, 3-fluorobenzonitrile, 2,3-difluorobenzonitrile, 2,4-difluorobenzonitrile and pentafluorobenzonitrile.

Measuring the rotational spectra of the parent molecules and the minor ^{13}C and ^{15}N isotopic species allowed the derivation of the substitution and effective structures for the studied molecules. While the substitution structures could not be accurately determined in most cases, a least-squares structural analysis resulted in more reliable effective structures. Using the effective and the calculated *ab initio* structures, the geometries of the fluorinated derivatives were compared to that of the reference compound (benzonitrile) and the effect of single, double and full fluorination on the geometry of benzonitrile was examined. The structural changes based on the effective structures, which were supported by the *ab initio* predictions, revealed that the partial and full fluorination distort the geometry of benzonitrile and such geometry changes can be monitored by the aid of the FTMW technique. The observed distortions in the BN geometry caused by single, double and full fluorination were interpreted by hybridization theory and intramolecular non-bonded interactions. To some extent, these effects seem additive for the multiply-substituted species.

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Chapter 1: Introduction

Studying the effect of substituents on the physicochemical properties of compounds is one of the long standing problems in chemistry. The substituents can have significant effects on the molecular geometry and electronic properties of a molecule via hybridization effects, resonance effects, intramolecular interactions, etc. [1]. When it comes to the molecular structure, the substituents usually cause small structural deformations however, tracking these small effects is possible with modern experimental and computational techniques [2] from which accurate molecular structures can be obtained.

Among the experimental techniques, microwave spectroscopy, known as rotational spectroscopy, is a valuable tool to accurately determine the molecular structure [3]. Using Fourier transform microwave spectroscopy, it is possible to study the molecules in the gas phase and at very low temperatures allowing one to measure the high resolution pure rotational spectrum of the isolated molecules in the ground vibrational state. In addition, the analysis of rotational spectra of the isotopic species allows one to specify the position of atoms in the molecule from which the structural parameters can be evaluated precisely within a few thousandths of Ångstroms for bond lengths and few tenths of degrees for bond angles and dihedral angles [2]. Such precision allows the monitoring of small distortions induced by the substitution of particular atoms.

In addition to microwave spectroscopy, computational chemistry tools can be used to investigate the effects of substitution. For instance, high level *ab initio* calculations give accurate equilibrium structures, which can complement the structures obtained from experimental techniques.

To study the structural deformations caused by substitution, there should be a suitable reference compound, for which the accurate molecular structure can be determined. The highly symmetric benzene molecule, as a suitable reference compound, and its substituted derivatives have been of great interest among chemists [4]. In fact, the distortion of the benzene ring upon substitution was studied extensively by different techniques including microwave spectroscopy, X-ray diffraction and computational chemistry [1,4-5]. For example, the fluorinated derivatives of benzene have been studied by the microwave spectroscopy and the deformation of benzene ring as a function of single, double and multiple fluorination was investigated [5-10]. From such investigations it was realized that a substituent can distort the benzene ring geometry by altering some of the ring bonds by up to 0.02 Å and some of the ring angles by up to 5°, which resulted in reducing the symmetry of the benzene ring.

Within the substituents, fluorine was one of the major interests. In fact, replacing the hydrogen with a fluorine atom can significantly affect the physical properties, chemical reactivity and biological activity of a compound. When it comes to structural studies, fluorine plays an important role as the structural deformations induced by fluorine substitution are expected to be at maximum due to its higher electronegativity compared to other atoms [11].

A number of fluorinated organic compounds have been studied using Fourier transform microwave spectroscopy in van Wijngaarden group at the University of Manitoba [12-18]. Among the studied compounds, the mono- and di-fluorinated pyridines which are shown in Figure 1.1, were investigated to realize the effect of fluorination on distortion of the aromatic ring in pyridine [14-15]. From those studies, it was found that the geometrical distortions caused by partial fluorination are efficient indicators of the interactions between the fluorine atoms and the pyridine ring backbone. Thanks to the Fourier transform microwave spectroscopy, small geometrical distortions of 0.006 Å for bond lengths and 0.6° for bond

angles could be monitored. Within such precision in studying the mono- and di-fluorinated pyridines, it was determined that the *ortho*-fluorinated derivatives showed a more pronounced deviation from the pyridine ring geometry. The observed distortions were then interpreted by a hyperconjugation model in which the electron density is donated from the fluorine's electron lone pairs into the π-system of pyridine [14-15] creating extra electron density near nitrogen.

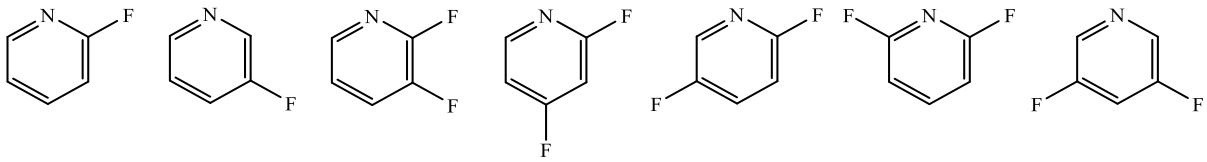

Figure 1.1: The studied mono- and di-fluorinated pyridines in van Wijngaarden group

In the current study, benzonitrile and some of its fluorinated derivatives are studied using Fourier transform microwave spectroscopy. The molecular structures of the studied compounds are illustrated in Figure 1.2.

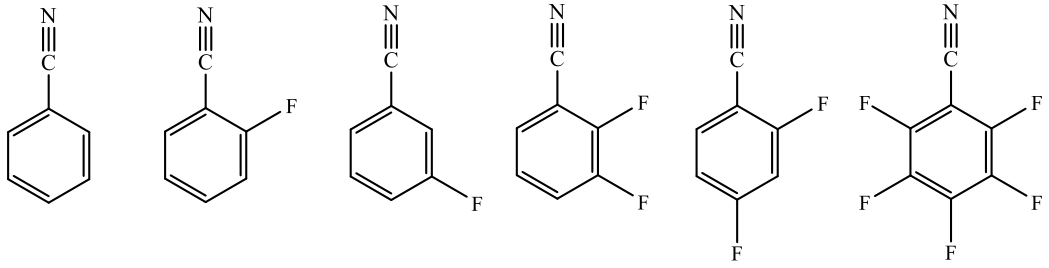

Figure 1.2: The studied molecules in the present thesis work. From left to right: benzonitrile, 2-fluorobenzonitrile, 3-fluorobenzonitrile, 2,3-difluorobenzonitrile, 2,4-difluorobenzonitrile, pentafluorobenzonitrile.

There are many fluorinated benzonitriles and the majority of them are commercially available. Therefore, there had to be strategic choices of the appropriate derivatives. The 2FBN and 3FBN derivatives were selected as the representatives of the mono-fluorinated benzonitriles for which the geometrical distortions follow a simple pattern, as there is only one fluorine atom in the molecular structure. The 23DFBN and 24DFBN were selected as

di-fluorinated benzonitriles; In 23DFBN, the two fluorine atoms are substituted in proximity whereas in 24DFBN, the fluorine atoms are not on neighbouring carbon atoms. In both 23DFBN and 24DFBN, due to the presence of two fluorine atoms, the additivity of effects may come into play in which some geometrical distortions may be caused by superimposing effects of the individual fluorine atoms. In PFBN, the geometrical distortions follow a more complex pattern as all the hydrogen atoms are substituted by fluorine. In this work, analysing the rotational spectra and determining the molecular structure of the studied benzonitriles allowed the investigation of the effect of partial and full fluorination on the geometry of benzene ring in benzonitrile.

In the following sections, some of the important concepts in rotational spectroscopy which have been utilized in the course of the present study are described.

1-1 What is rotational spectroscopy?

Rotational spectroscopy is a technique which utilizes the microwave region of the electromagnetic radiation to measure the energies of rotational transitions of molecules in the gas phase. The various forms of the electromagnetic radiation are shown in Figure 1.3 from which it is seen that the microwave region has relatively large wavelength and low frequency which is extended from 1 to 1000 GHz [3].

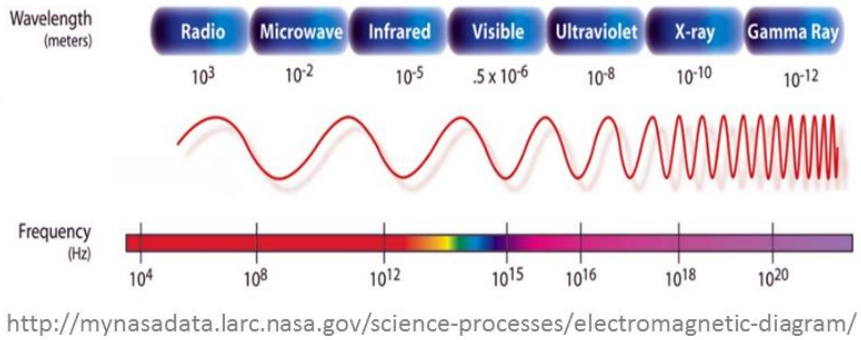

Figure 1.3: Different regions of electromagnetic radiation

The incident microwave radiation can excite the rotational energy levels of the molecules provided there is a permanent electric dipole moment in the molecule. Once the molecules are rotationally excited, the spectral transitions are measured and then used to describe the rotational energy levels of the molecule.

1-2 Moment of inertia

One of the key concepts in rotational spectroscopy is the moment of inertia, which is defined as "the mass of each atom multiplied by the square of its distance from the rotational axis through the center of mass of the molecule" [19] and is calculated by the formula $I = \sum_i m_i r_i^2$ where r_i is the distance of atom *i* to the rotation axis. There are three moments of inertia I_a, I_b and I_c which account for the rotation of molecule around the three perpendicular axes *a*, *b* and *c*. The molecules can be classified in four groups based on the values of moments of inertia [20]:

i) Linear rotors for which $I_b = I_c$ and $I_a = 0$; have one unique moment of inertia,

ii) Spherical rotors for which $I_a = I_b = I_c$; have three equal moments of inertia,

iii) Symmetric rotors for which $I_a < I_b = I_c$ (prolate symmetric top) or $I_a = I_b < I_c$ (oblate symmetric top); have two equal moments of inertia,

iv) Asymmetric rotors for which $I_a < I_b < I_c$; have three different moments of inertia.

Another key molecular parameter is the rotational constant which is inversely related to the moment of inertia. There exist three rotational constants and are expressed as [20]

$$A=\frac{h}{8\pi^2 I_a} \quad , \quad B=\frac{h}{8\pi^2 I_b} \quad , \quad C=\frac{h}{8\pi^2 I_c} \qquad \text{Eq. 1.1}$$

All the molecules in this study are asymmetric rotors and therefore have three different moments of inertia I_a, I_b and I_c and different values for the rotational constants A, B and C where A > B > C.

By analysing the rotational spectra, it is possible to evaluate the rotational constants A, B and C, from which the molecular structures can be evaluated. The structural information can be obtained from the moments of inertia which are derivable from the rotational constants using Eq. 1.1. The rotational constants of the isotopically-substituted species are usually required to derive the structural parameters including the bond lengths, bond angles and dihedral angles [3].

1-3 Rotational energy-level expression

Different types of rotors have their own energy expressions to describe the rotational energy levels and are obtained from solving (or approximately solving) the Schrödinger equation. The rotational energy expressions for different types of rotors are as follow [19]

Linear or spherical tops:

$$F(J) = BJ(J+1) \quad J=0, 1, 2, \ldots \qquad \text{Eq. 1.2}$$

Symmetric top, prolate rotor:

$$F(J,K) = BJ(J+1) + (A-B)K^2 \quad J=0, 1, 2, \ldots \quad K=0, \pm1, \ldots, \pm J \qquad \text{Eq. 1.3}$$

Symmetric top, oblate rotor:

$$F(J,K) = BJ(J+1) + (C-B)K^2 \quad J=0, 1, 2, \ldots \quad K=0, \pm1, \ldots, \pm J \qquad \text{Eq. 1.4}$$

In these equations, F(J) is called the rotational term value which is used to express the energy of a rotational state and has the unit of either wavenumber (cm^{-1}) or frequency (Hz). The J and K are quantum numbers in which J is the magnitude of the angular momentum of the molecule and K represents the component of the angular momentum J along the principal axis.

The rotational energy-level expressions for linear, spherical and symmetric tops are obtained from the analytical solution of the Schrödinger equation however, there is no general analytical solution for asymmetric tops [3]; In fact, for asymmetric rotors, the Schrödinger equation must be solved numerically by a computer. The rotational energy levels are then labeled based on the prolate-oblate correlation diagram [20] which is shown in Figure 1.4.

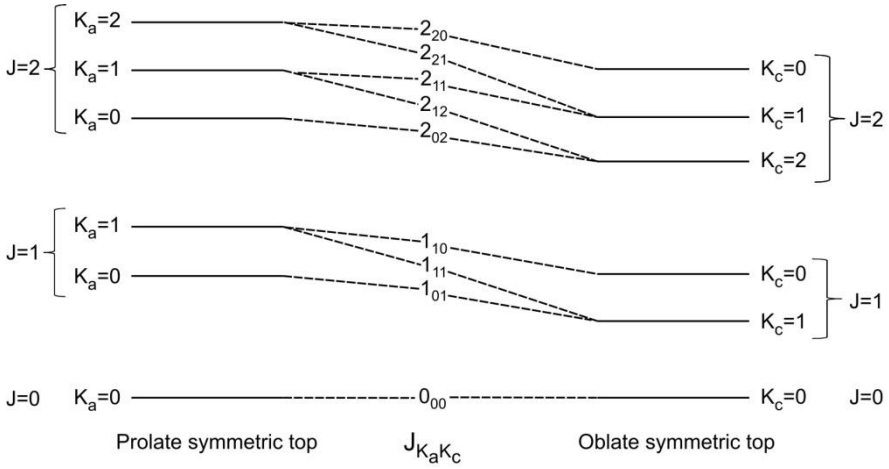

Figure 1.4: Correlation diagram for prolate and oblate symmetric tops

According to Figure 1.4, the rotational energy levels of an asymmetric rotor are denoted by $J_{K_aK_c}$ notation in which J is the angular momentum and K_a and K_c are used to label the rotational energy levels. It is seen that the rotational energy levels for asymmetric rotors have a more complex pattern than those for prolate and oblate rotors.

1-4 Centrifugal distortion

In deriving the energy expression for the rotational energy levels of different rotors (equations 1.2 to 1.4), it was assumed that the molecules are rigid rotors however, in practice the molecules are not rigid and the atoms in real molecules move around their equilibrium positions. As a molecule is rotating, the centrifugal forces distort the molecular geometry which cause a change in the moment of inertia. For instance, in a diatomic molecule, as the molecule rotates faster, i.e. as J increases, the bond is more stretched which leads to an increase in the moment of inertia and consequently a decrease in the rotational constant B [21]; Therefore in a non-rigid diatomic molecule, the rotational energy levels are slightly closer together than in a rigid diatomic molecule [19].

Considering the centrifugal distortions and their effect on the rotational energy levels, some corrections need to be added to the rotational energy-level expressions to account for those distortions. For the molecules in this study, which are all asymmetric rotors, five centrifugal distortion constants are considered including Δ_J, Δ_K, Δ_{JK}, δ_J and δ_K parameters [3]. These centrifugal distortion constants are used to account for the departure of actual rotational transitions from the ideal rigid model predictions. The centrifugal distortion parameters thus give information about the rigidity of the molecule and small magnitudes of such constants correspond to a more rigid molecular structure.

1-5 Rotational selection rules

The selection rules are a set of conditions which determine which rotational transitions are allowed (observable) for a molecule. As a general selection rule, there must be a permanent electric dipole moment in the molecule to show the rotational spectrum [19]. In addition to

this general condition, the components of dipole moment on the principal axes *a*, *b* and *c* specify the type of rotational transitions as follow [20]

1) *a*-type transitions: which are observed when μ_a has a non-zero value and have the selection rules $\Delta J=\pm1$, $\Delta K_a=0, \pm2, \ldots$ and $\Delta K_c= \pm1, \pm3, \ldots$

2) *b*-type transitions: which are observed when μ_b has a non-zero value and have the selection rules $\Delta J=\pm1$, $\Delta K_a=\pm1, \pm3, \ldots$ and $\Delta K_c= \pm1, \pm3, \ldots$

3) *c*-type transitions: which are observed when μ_c has a non-zero value and have the selection rules $\Delta J=\pm1$, $\Delta K_a=\pm1, \pm3, \ldots$ and $\Delta K_c= 0, \pm2, \ldots$

All the molecules in this thesis (Figure 1.2) have a permanent electric dipole moment and hence there are some allowed rotational transitions for them. Within the studied molecules, some show only *a*-type transitions and some show both *a*- and *b*-type transitions. None show *c*-type transitions because the μ_c dipole component of the studied molecules is zero.

1-6 Nuclear quadrupole hyperfine structure

Nuclear quadrupole hyperfine structure is a type of splitting in the rotational energy levels which is observed for molecules involving nuclei with the nuclear spin quantum number $I > \frac{1}{2}$ [22]. Such splitting originates from the interaction between the nuclear quadrupole moment and the molecular electric field gradient. As a result of this interaction, a coupling between the nuclear spin I and the molecular rotational angular momentum J happens to give the total angular momentum F [3]. For an asymmetric rotor involving a nucleus with nuclear spin $I > \frac{1}{2}$, in addition to the quantum numbers J, K_a and K_c, the forth quantum number F is required to describe the energy levels where the quantum number F accounts for the splitting in the rotational spectrum.

The analysis of nuclear quadrupole hyperfine structure is a useful tool to study the electronic structure around the quadrupolar nucleus. The hyperfine splitting in the rotational spectrum

ranges from few kHz to few MHz depending on the magnitude of the nuclear quadrupole moment [22]. All of the molecules in this study contain the ^{14}N nucleus which has the nuclear spin I = 1 and therefore all show the hyperfine splitting in their rotational spectra which is in the order of few KHz.

In summary to this chapter, being aware of the important concepts in rotational spectroscopy, as presented in sections 1-1 to 1-6, helps characterize the rotational properties of compounds. In fact, by analysing the rotational spectrum of a molecule, it is possible to evaluate the spectroscopic constants including rotational constants (A, B and C), centrifugal distortion parameters and nuclear quadrupole coupling constants. From the rotational constants, the moments of inertia are extracted which are functions of interatomic distances. Eventually, using the moments of inertia (or rotational constants) of a molecule and the slightly departed values for the minor isotopic species, the molecular structure can be evaluated.

The rest of this thesis work is presented as five chapters. Chapter 2 describes the instruments and methodologies used in the current study. In Chapter 3, the results of microwave studies and structural determination for symmetric benzonitriles including benzonitrile and pentafluorobenzonitrile are presented and the effect of full fluorination on the geometry of benzonitrile is discussed. Chapter 4 is dedicated to the microwave studies and structural determination for mono-fluorinated benzonitriles including 2-fluorobenzonitrile and 3-fluorobenzonitrile and the effect of single fluorine substitution at the *ortho* and *meta* positions on the benzonitrile geometry is described. In Chapter 5, the results of microwave studies and structural determination for di-fluorinated benzonitriles including 2,3-difluorobenzonitrile and 2,4-difluorobenzonitrile are presented and the effect of double fluorine substitution on the geometry of benzonitrile is discussed. In Chapter 6, general conclusions are drawn for this thesis work and some possible future studies as extension to the current research are described.

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Chapter 2. Instrumentation and methods

Studying the rotational spectra and structures of benzonitrile and its fluorinated derivatives was not possible without using the appropriate facilities. In this chapter, the instruments and methodologies which have been used in the current research are introduced.

2-1 Instrumentation

To collect the MW spectra of benzonitrile and its fluorinated derivatives, two types of custom-built Fourier transform microwave (FTMW) spectrometers were used including the Balle-Flygare FTMW and Chirped-Pulse FTMW (cp-FTMW) instruments. Both instruments have common characteristics, e.g. using the pulsed supersonic jet expansion, while they are different mainly due to utilizing different electronic components for excitation and detection operations. In the following sections, the common features of the two instruments are described and then each instrument is presented individually.

2-1-1 An overview of Fourier transform microwave spectroscopy

The overall scheme of the FTMW technique is shown in Figure 2.1. A mixture of the vapour pressure of the sample and a carrier gas is sent through a pulsed nozzle. The carrier gas is chosen to be a noble gas. The nozzle pulses the gas mixture into a chamber evacuated to a pressure of ~10^{-6} Torr. A molecular beam is generated as a result of the supersonic expansion of the gas at the nozzle in which the molecules in the beam are rotationally cooled down to few degrees Kelvin. Shortly after the gas is pulsed, the MW pulses are broadcasted into the cavity. If the sample molecules have rotational transitions within the range of the incident MW radiation, the molecules will be polarized and rotated coherently. Once the radiation is turned off, the rotationally excited molecules will produce their own time-

diminishing emission signals which are recorded as free induction decays, FIDs. The FIDs are then Fourier transformed to obtain the frequency domain spectrum.

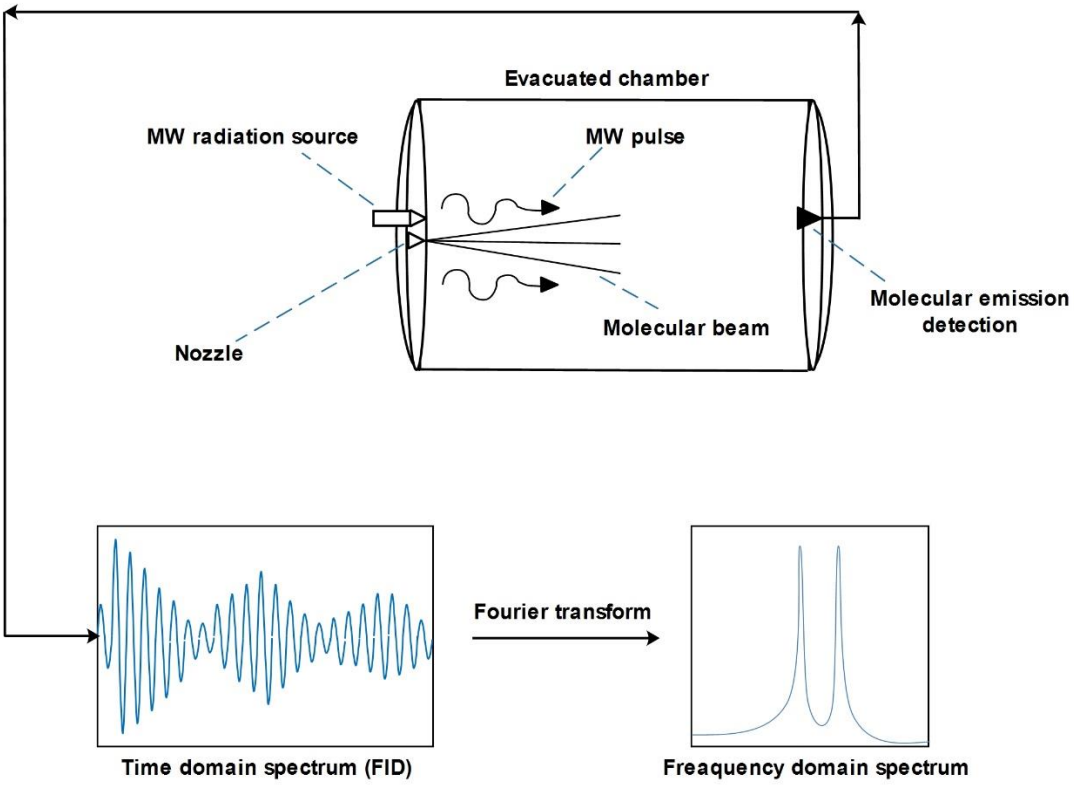

Figure 2.1: The schematic of the FTMW spectroscopy

2-1-2 Pulsed supersonic expansion

The supersonic expansion is a process during which a gas at a higher pressure is pulsed into an evacuated chamber through a fast solenoid valve called a nozzle [1]. A typical nozzle is shown in Figure 2.2.

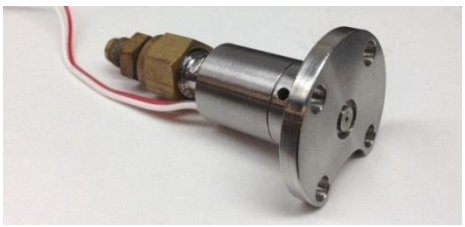

Figure 2.2: A solenoid valve nozzle

A noble gas is used to carry the desired sample towards the nozzle. Once the supersonic expansion happens at the nozzle, a molecular beam is created and since there is no heat exchanged between the gas molecules in the beam and the chamber, the supersonic expansion is an adiabatic process [2].

The carrier gas is chosen to be a monoatomic noble gas having only translational degrees of freedom. As a result of the adiabatic expansion, the translational temperature of the carrier gas, which is a function of the velocity distribution of the gas particles in the beam, is effectively decreased to few degrees Kelvin. In other words, the carrier gas molecules in the beam are moving with almost the same velocities and there is a narrow distribution of velocities among the beam particles which cause a drastic decrease in translational temperature of the carrier gas [3].

During the supersonic expansion, the polyatomic molecules (of the desired sample) collide with the translationally cooled atoms of the carrier gas via two-body collisions. As a result, the translational temperature of the polyatomic molecules is cooled to comparably low temperatures. The rotational and vibrational temperatures, which are measures of the distribution of particles over the rotational and vibrational energy levels, are cooled as well. Between the rotational and vibrational temperatures, the rotational cooling is done more efficiently since the gap between the rotational energy levels is much smaller than that of the vibrational energy levels [3].

The reduction of rotational and vibrational temperatures is the key benefit to the molecular beams especially when it is coupled to the FTMW technique. Since the molecules occupy the lowest rotational energy levels, the low lying rotational transitions become stronger while the transitions due to higher levels are weakened. This will lead to more sensitivity in the

technique and a more simplified spectrum than that obtained from the room-temperature wave-guide MW spectroscopy [4].

There is a collision-free environment in the supersonic jet which leads to more resolution in the MW spectrum. Due to the collision-free medium, major sources of spectral broadening are removed; The pressure broadening is avoided and also the Doppler broadening is minimized since there is a narrow distribution of velocities among the particles moving in the molecular beam. The collision free medium also allows the study of unstable and short-lived species, e.g. ions and radicals. It is worth mentioning that although the Doppler broadening is reduced while using molecular beams, however there may be a Doppler splitting in the MW spectrum if the microwave pulses are radiated parallel to the molecular beam as the emitting molecules are moving while the receiving antenna is stationary [4].

2-1-3 Balle-Flygare FTMW instrument

The cavity FTMW spectrometer at University of Manitoba is shown in Figure 2.3 which was used throughout the experiments described in this thesis. It is a custom-built FTMW instrument assembled in van Wijngaarden's lab [5] and its operating principles are the same as described by Balle and Flygare [6].

Some general characteristics of the FTMW technique were described in Sections 2-1-1 and 2-1-2 and the two specific components of the Ball-Flygare FTMW spectrometer, which are the cavity and electronic circuit, are described here. For the sake of ease, the Balle-Flygare FTMW spectrometer will be stated briefly as FTMW instrument.

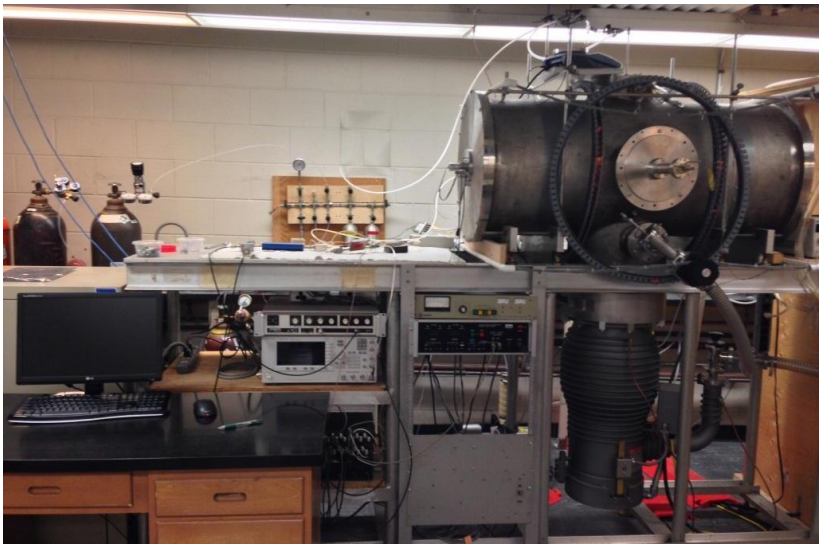

Figure 2.3: The Balle-Flygare FTMW instrument at the University of Manitoba

2-1-3-1 Fabry-Pérot cavity

The Fabry-Pérot cavity consists of two concave aluminum mirrors which are 35.6 cm in diameter and approximately 65.0 cm far apart and is shown in Figure 2.4. The cavity is placed in a chamber evacuated to a pressure of ~10^{-6}. Adjusting the distance between the two mirrors allows the cavity to be tuned to a desired frequency between 4 to 26 GHz.

The high vacuum inside the chamber is achieved by a diffusion pump (Varian VHS-10) with the pumping speed of 3650 $L.s^{-1}$ and a rotary pump (Edwards E2M80).

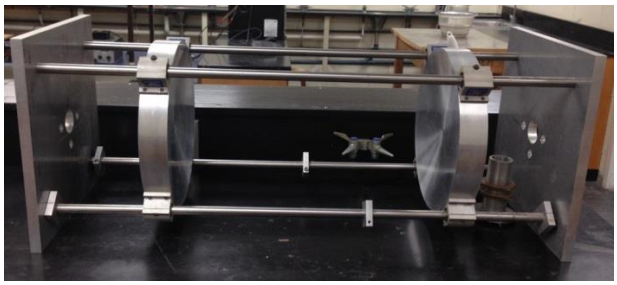

Figure 2.4: The concave aluminum mirrors of the Fabry-Pérot cavity

2-1-3-2 The FTMW spectrometer circuit

The electronic circuit of the FTMW instrument is illustrated in Figure 2.5.

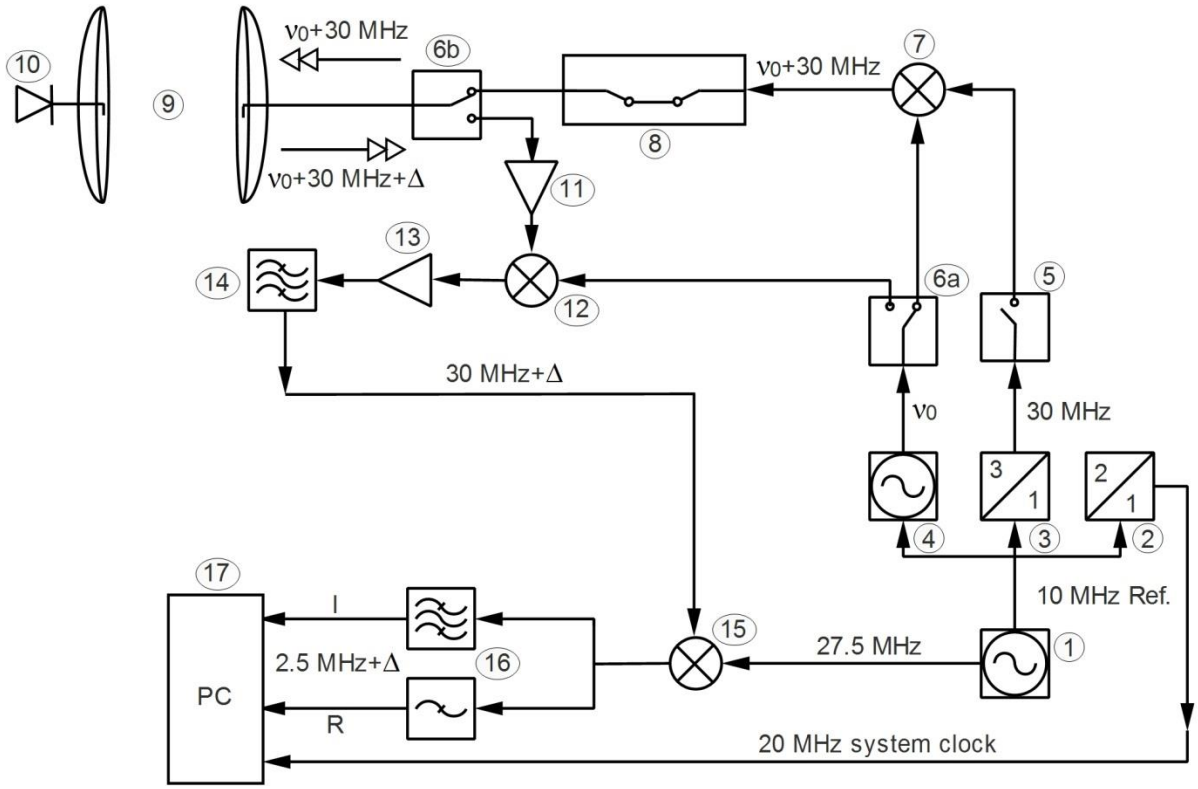

Figure 2.5: The electronic circuit of the Balle-Flygare FTMW instrument: (1) RF synthesizer, (2) Doubler, (3) Tripler, (4) MW synthesizer, (5) SPDT GaAs RF switch, (6) SPDT *p-i-n*-diode MW switch, (7) Single sideband mixer, (8) Coaxial transfer switch, (9) Fabry-Pérot cavity, (10) Diode detector, (11) Low noise amplifier, (12) Image rejection mixer, (13) RF amplifier, (14) Bandpass filter, (15) RF demodulator, (16) Lowpass filter, (17) Two-channel transient recorder.

A microwave pulse is provided by a microwave synthesizer (4) and two *p-i-n* diode SPDT switches (6a,6b). The length of the pulse is chosen to be between 1 to 4 μs and is adjusted to achieve the highest S/N ratio when tuned to a molecular transition. The microwave synthesizer generates the frequency ν_0 which is 30 MHz below the desired excitation frequency while the remaining 30 MHz is compensated by combining the frequency ν_0 and the tripled output of the 10 MHz reference through the single sideband mixer (7). The doubled output of the 10 MHz reference is used to synchronize the electronic components and to adjust the timings for pulses and delays. The incident MW pulse at ν_0+30 MHz is then coupled into the cavity (9) through the antenna mounted in the center of the moving mirror

while a diode detector (10) ensures the resonance in the cavity. If the incident MW radiation rotationally excites the sample molecules, the molecular emission signal at the frequency of ν_0+30 MHz+Δ is observed in which Δ is the difference between the actual rational transition frequency and the tuned excitation frequency. The free induction decays (FIDs) are received as a current in the antenna (mounted inside the moving mirror) which is then amplified using a low noise amplifier (11). The obtained molecular transition signal lies in the microwave frequency domain and in order to be feasibly digitized, it should be downconverted into the lower radiofrequency region. The first downconversion happens by removing the ν_0 frequency from the emission signal using the image rejection mixer (12). The downconverted signal is in the RF range and is amplified (13) and is passed through a bandpass filter (14) which selectively transmits the defined portion of the spectrum. The 30 MHz+Δ emission signal is then combined with the 27.5 MHz output of the radiofrequency synthesizer (1) in a RF demodulator (15) so that the signal can be transformed into a usable form. The 2.5 MHz+Δ signal is digitized by the aid of a two-channel transient recorder card which is embedded in a personal computer (17). The digitized time domain signal is then Fourier transformed to obtain the frequency domain spectrum. The cavity and also all pulses and delays are controlled by the FTMW++ program [7].

2-1-3-3 Timing

Figure 2.6 illustrates the important timings for a typical MW experiment on FTMW instrument. By adjusting theses timings it is possible to achieve the optimum (S/N) while measuring the rotational transitions.

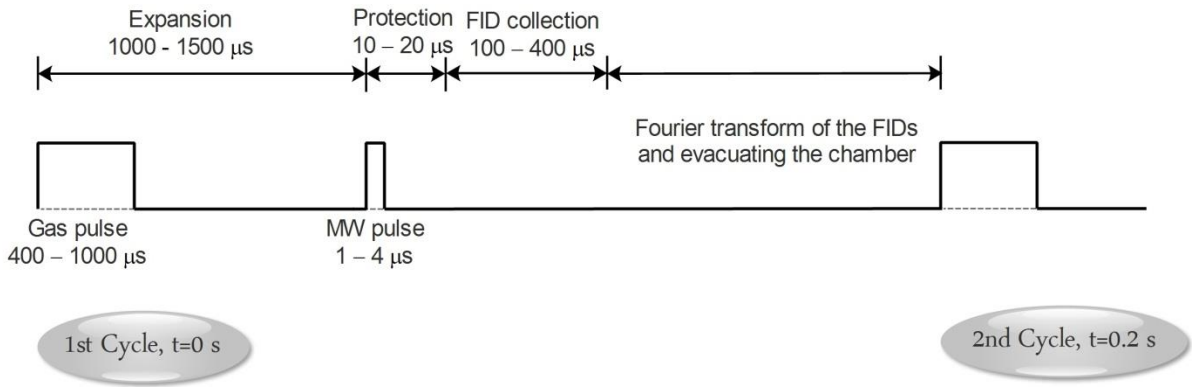

Figure 2.6: Time durations for a MW experiment

In Figure 2.6, it is assumed that the operation frequency is 5 Hz which means 5 whole experiments (each including excitation and detection steps) happen in 1 second and therefore the time length for each experiment (cycle) will be 0.2 s.

An experiment starts with a gas pulse taking 400 to 1000 µs. The gas pulse is allowed to adiabatically expand for few hundred microseconds. The expansion time, which takes 1000 to 1500 µs, specifies the total time needed for pulsing the gas and the following expansion. Right after the expansion stage, a MW pulse (with a desired frequency) is broadcasted into the cavity for 1 to 4 µs. Simultaneous to the MW pulse, the detection part of the circuit is protected from receiving the MW pulse for 10 to 20 µs to make sure the incident radiation in the cavity decays and only the molecular emission signal will be collected. Right after, the FID is recorded for 100 to 400 µs. The rest of the time in the cycle is used to perform the Fourier transform and to evacuate the chamber so that it is ready for the next cycle. The FIDs recorded from each cycle can also be averaged and transformed to accumulate a spectrum over many cycles.

2-1-4 Chirped pulse FTMW instrument

The Chirped Pulse FTMW (cp- FTMW) technique was first developed by Brooks H. Pate and co-workers in 2008 [8]. The custom built cp-FTMW instrument of the van Wijngaarden's lab

at the University of Manitoba [9] is shown in Figure 2.7 and was used for some experiments in the current study.

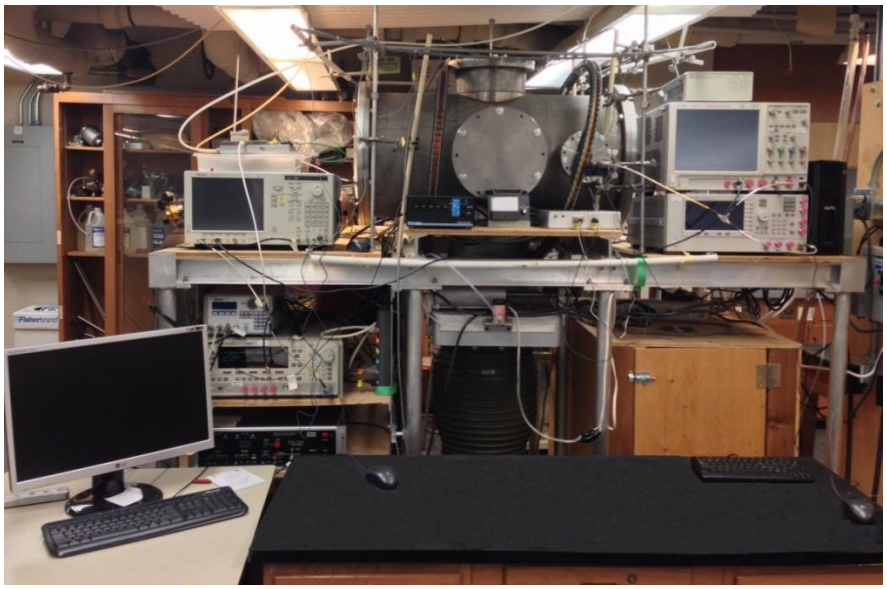

Figure 2.7: The cp-FTMW instrument at the University of Manitoba

In contrast to the FTMW instrument, the cp-FTMW device is able to cover a wide region of the MW spectrum, from few MHz to few GHz, in a single data acquisition. The broadband capability of the cp-FTMW instrument is due to the unique electronic circuit which utilizes the advantages of an arbitrary waveform generator and the broadband digitizing oscilloscope [8].

2-1-4-1 The cp-FTMW spectrometer circuit

The microwave circuit for the cp-FTMW instrument is shown in Figure 2.8. An arbitrary waveform generator (1) produces a chirped pulse which is mixed with a fixed frequency output of a microwave signal generator (3a) in a double balanced mixer (4). The produced MW excitation pulse is an ultrafast linear frequency sweep and is centered at the output frequency of the MW signal generator. The generated excitation pulse has an adjustable ban-

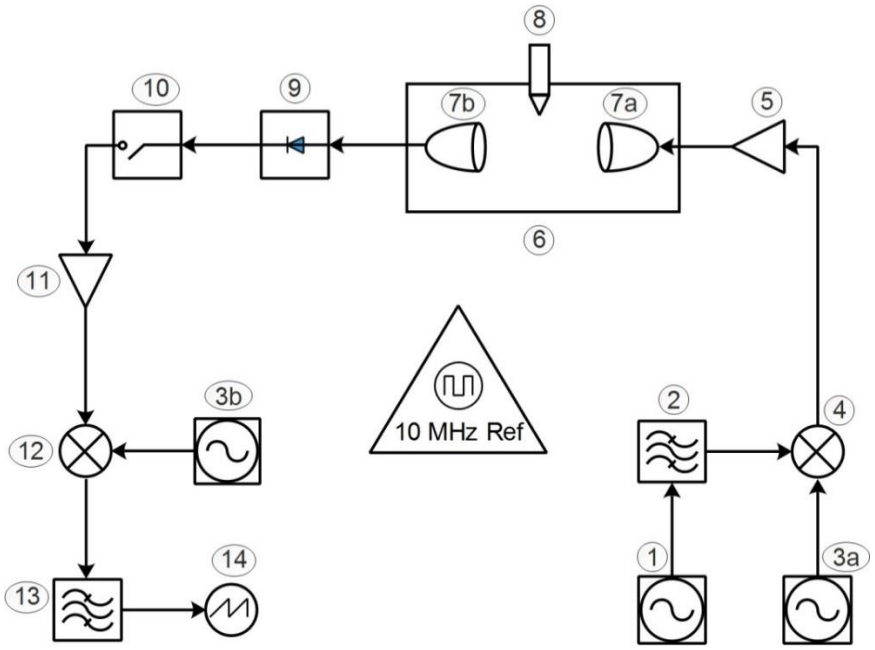

Figure 2.8: The electronic circuit of cp-FTMW instrument: (1) Arbitrary waveform generator (6 GSa/s), (2) Low pass filter, (3) Microwave signal generator, (4) Double balanced mixer, (5) Solid state amplifier (5W), (6) Chamber, (7) Horn antennas, (8) Supersonic nozzle, (9) Diode limiter, (10) SPST switch, (11) Low noise amplifier, (12) Triple balanced mixer, (13) Low pass filter/DC block, (14) Digital oscilloscope.

-dwidth of up to 6 GHz and has to be amplified (5) before being broadcasted into the chamber (6) through a horn antenna (7a). A diffusion pump (Varian VHS 10) and two rotary pumps (Varian DS602) evacuate the camber to a pressure of ~10^{-6} Torr. The gaseous sample is pulsed into the chamber via a nozzle (8). To protect the detection branch of the circuit from receiving the polarizing pulse, a high-power *p*-*i*-*n* diode (9) is used ahead of the SPST switch (10). Once the excitation pulse is dissipated, the broadband molecular emission (FID) is received in the horn antenna (7b) and is amplified by a low noise amplifier (11). The amplified emission signal is then downconverted to a lower frequency range for digitization which is accomplished by another microwave signal generator (3b) and a mixer (12). The downconverted emission signal is passed through a filter (13) and FIDs are digitized by a digital oscilloscope (14). A 10 MHz reference clock is used to synchronize the electronic components and all pulses and delays.

2-1-4-2 Timing

A typical MW experiment on cp-FTMW instrument, similar to that using the FTMW device, is conducted by adjusting the timings for the gas pulse and MW excitation/detection operations. Theses timings are chosen to achieve the highest S/N ratio in the course of measuring the rotational transitions.

The operation frequency is 5 to 10 Hz which means 5 to 10 whole experiments happen in 1 second and the time duration for each cycle is 0.1 to 0.2 s. The experiment initiates when the gas is pulsed for 400 to 1000 μs. The expansion step takes 1000 to 1500 μs which involves the gas pulse duration and the following adiabatic expansion. Shortly after the expansion, the broadband MW excitation pulse with a desired bandwidth is broadcasted into the chamber for 1 to 4 μs. Once the MW radiation is turned off, the molecular emission signals, FIDs, are recorded 1 to 20 μs. The remaining time of the cycle is used for the fast Fourier transformation of FIDs and restoring the vacuum in the chamber. It is usually desired to average the FIDs over many cycles to improve the S/N ratio.

2-1-5 Comparing FTMW and cp-FTMW instruments

Choosing the proper MW spectrometer depends on the goals of study and also the extent of MW research that has previously been done on the molecule of interest. Being aware of advantages and disadvantages of the two MW spectrometers makes it easier to select the right device(s) to work.

The two key advantages to the FTMW instrument are the higher sensitivity and higher resolution in the MW spectrum which arise from using the cavity. The use of cavity in the FTMW instrument makes it a narrowband spectrometer to cover only ~1 MHz of the MW spectrum at a time. Therefore, the power of the MW pulse is concentrated in a narrow bandwidth which consequently leads to the less power requirements for the MW excitation

pulse while the amplitude of the emission signal is enhanced [8]. The high resolution of the FTMW instrument makes it possible to study the small effects, e.g. the hyperfine structure and the increased sensitivity leads to a greater S/N ratio which is especially important while searching for the minor isotopologues' transitions [4].

On the opposite side, the FTMW instrument is a time-consuming device due to the use of the cavity; For measuring a rotational transition, the cavity needs to be physically tuned to the corresponding frequency and once that transition is measured, the cavity position needs to be tuned again for the next transition frequency which eventually makes it tedious for the fast acquisition of a spectrum [4].

The main advantage to the cp-FTMW instrument is the broadband capability which allows the collection of a wide range of the MW spectrum for each gas pulse. The broadband performance eventually leads to a reduction in the measurement time and sample consumption and therefore, the cp-FTMW device is the proper instrument for the initial MW studies of the molecules [8]. The cp-FTMW instrument also does not possess the moving parts which makes it easier to work with.

The disadvantage of the cp-FTMW spectrometer is the lower sensitivity and resolution because of two reasons: 1) it lacks the cavity and 2) the cp-FTMW device covers several MHz or GHz of the spectrum in each MW pulse and hence, the power is distributed over a broadband pulse [8]. Therefore, it is not the proper choice to study the small effects, e.g. the hyperfine splitting and weak emission signals.

2-2 Methods

To do a microwave study of a new molecule, in addition to collecting data using the MW spectrometers, a wide variety of methods are applied to analyze the rotational spectrum and to obtain the molecular geometry which are briefly described here.

2-2-1 Handling the spectrum

The measured rotational frequencies from the MW spectrometer are initially fitted to a Hamiltonian model using the Pickett's SPFIT program [10] which is a general least-squares fitting routine employed for rotationally resolved spectra of all types. In least-squares fitting, the sum of squared residuals are minimized where a residual is the difference between the observed rotational frequency and the predicted frequency by the Hamiltonian model employed [11]. For asymmetric rotors, the Hamiltonian model is normally chosen to be the Watson's A-reduced Hamiltonian (I^r representation) [12]. From this fitting, the approximate values of the spectroscopic constants including the rotational constants (A, B and C), centrifugal distortion parameters and the nuclear quadrupole coupling constants are obtained. The results of the SFPIT program are used to predict a new list of transitions using the Pickett's SPCAT program [10] which allows for extensions of the range of measurements. The new transitions are then measured and added to the spectral fit until the Hamiltonian parameters are well determined in both sign and magnitude.

2-2-2 Evaluation of the molecular structure

Two types of the experimental structures are evaluated for the molecules in this study: the substitution structure and the effective structure. For this purpose, the rotational constants (A, B and C) of the parent molecule and its minor isotopologues are required as input.

To evaluate the substitution structure, a Kraitchman analysis [13] is performed in which the position of each atom in the molecule is calculated according to the change in the moments of inertia as a result of a single isotopic substitution at various sites in the molecule [14]. The KRA program [15] is used to do the Kraitchman analysis which gives the absolute values of the atomic Cartesian coordinates from the axes of rotation while the uncertainties in the coordinates are calculated from Costain's rule [16]. The Cartesian coordinates and their uncertainties are converted into the internal coordinates and their uncertainties using the EVAL program [15] from which the values of bond lengths, bond angles, and dihedral angles can be extracted. The substitution structural parameters are denoted by r_s in which s denotes the term substitution.

To obtain the effective structure, a least-squares approach is used. To do the least-squares analysis, the STRFIT program [15] is used. The STRFIT program fits the ground state rotational constants for all isotopologues to key internal structural parameters in order to reproduce the experimental moments of inertia [14]. The fitted structural parameters with their uncertainties are then obtained from the least-squares analysis. The effective structural parameters are shown by r_0 which 0 refers to the ground vibrational state.

In addition to the experimental structures, the equilibrium structure is estimated with the *ab initio* calculations performed by the Gaussian 09 program [17]. All the geometry optimizations are performed at MP2/6-311++G(2d,2p) level of theory. Additional electron correlation effects are considered by using the second-order Møller–Plesset perturbation theory and when this method is coupled to a large basis set [6-311++G(2d,2p) in this case], it can give reliable results comparable to the experiment. The calculated equilibrium structure is shown by r_e which can be used as the initial structural coordinates to be used as input with the STRFIT program.

2-3 A typical MW experiment

The starting point of a microwave study depends on how much work has previously been done on a parent molecule and its minor isotopic species. For the following description, it is assumed that there have been no microwave studies on the molecule of interest.

First of all, the equilibrium geometry of the molecule is calculated using an *ab initio* method with a large basis set at the MP2/6-311++G(2d,2p) level of theory. Having the calculated rotational constants (A, B and C) and the estimated values of dipole moment components, the SPCAT program generates a list of predicted transition frequencies with their intensities. Some of the strong transitions between 8 to 18 GHz are considered and the cp-FTMW instrument is used to collect a broadband spectrum around the predicted frequencies. Once a few strong transitions are recorded, their corresponding quantum numbers are assigned and they are initially fitted to Watson's A-reduced Hamiltonian (I^r representation) model [12]. The results of the preliminary fit are used to generate a more precise prediction list.

The next stage is to move to the Balle-Flygare FTMW instrument. This instrument provides a higher resolution MW spectrum showing more details about the rotational transitions, for example, the nuclear quadrupole hyperfine structure which is observable for the molecules in this study due to the presence of a quadrupolar ^{14}N nucleus. The observed low resolution rotational transitions from the cp-FTMW instrument are reinvestigated using the FTMW device and the more precisely measured transitions are included in the fit to get improved values for the spectroscopic constants. If the rotational spectrum includes hyperfine structure, the additional nuclear quadrupole coupling constants may be included in the fit to account for the hyperfine splitting. The high resolution measurements are continued until as many transitions between 4 to 26 GHz are collected as possible and fitted. The Hamiltonian parameters should be well determined and physically meaningful.

To study the minor isotopic species, both the cp-FTMW and FTMW instruments can be used independently. While using the cp-FTMW spectrometer, since the minor isotopologue transitions are weak due to small natural abundance, some of the parent's strong transitions are chosen and the experimental settings are optimized to achieve the highest S/N ratio. The cp-FTMW is then set to operate for 60,000 cycles such that the weak transitions due to the minor isotopologues are observed. Those weak transitions are assigned with the proper quantum numbers and are then re-measured with the FTMW instrument to be included in their corresponding fits.

It is also possible to measure the rotational spectrum of the isotopic species only by using the FTMW instrument. To do so, the scaled rotational constants for the isotopologues are calculated using the PMIFST program [15] and their corresponding frequency lists are generated by the SPCAT program. Then, the spectrum of a strong parent transition is optimized to achieve the highest S/N ratio. Since the frequency predictions for the minor isotopologues are not precise at this stage, a small region surrounding the predicted frequencies is scanned so that a few MHz (often up to 5 MHz) above and below the anticipated frequency is covered. For instance, if the predicted rotational transition for a certain minor isotopologue is to be at 8000 MHz, 5 MHz above and below this value (7995 MHz to 8005 MHz) is scanned in incremental steps of 0.2 MHz. In this example, it takes 51 steps to cover the mentioned 10 MHz range while the cavity needs to be tuned for each step. Once a weak transition is found, the FTMW instrument averages the spectrum until the hyperfine structure is resolved. This process is continued until sufficient number of transitions for the isotopic species is obtained and the parameters in their corresponding fits are well determined.

Once the spectral fittings for the parent molecule and minor isotopologues are accomplished, it is time to evaluate the experimental structures. The substitution (r_s) structure is evaluated

using the KRA/EVAL programs and the effective (r_0) structure is obtained from the STRFIT program. The whole process for a typical MW experiment is summarized in Figure 2.9.

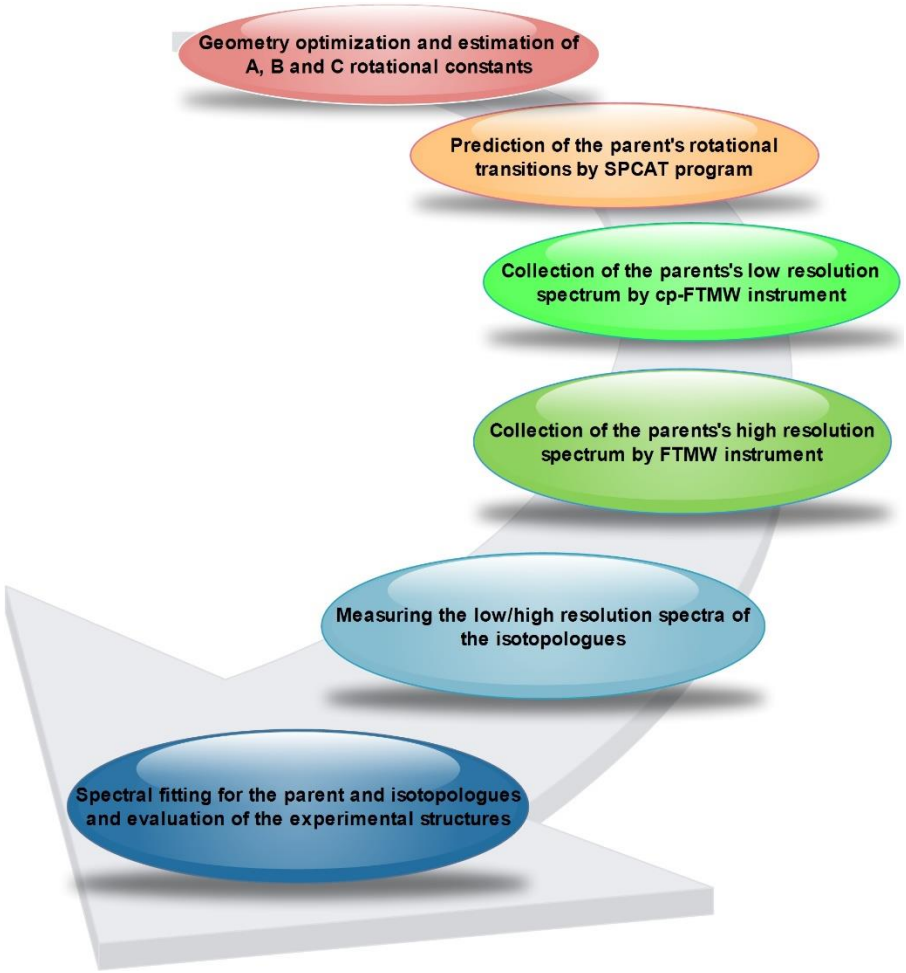

Figure 2.9: Different steps of a typical MW experiment

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Chapter 3: Microwave study and molecular structure of benzonitrile and pentafluorobenzonitrile

The first studied molecules in the current research are the symmetric molecules including benzonitrile (BN) and pentafluorobenzonitrile (PFBN). BN is chosen to be the reference compound and its geometry changes via full fluorination are examined. The results of the MW investigations and structural determinations for BN and PFBN are presented here and the effect of full fluorination on the geometry of BN is discussed.

3-1 Introduction

The molecular structures of BN and PFBN and their principal axis systems are shown in Figure 3.1 and Figure 3.2. Both molecules are asymmetric rotors with the point group of C_{2v}. The dipole moment of BN is experimentally evaluated to be 4.51 D [1] while that of PFBN is estimated to be 2.79 D [at MP2/6-311++G(2d,2p) level of theory]. The dipole moments are aligned towards the *a* principal inertial axis and therefore strong *a*-type transitions are expected for both molecules.

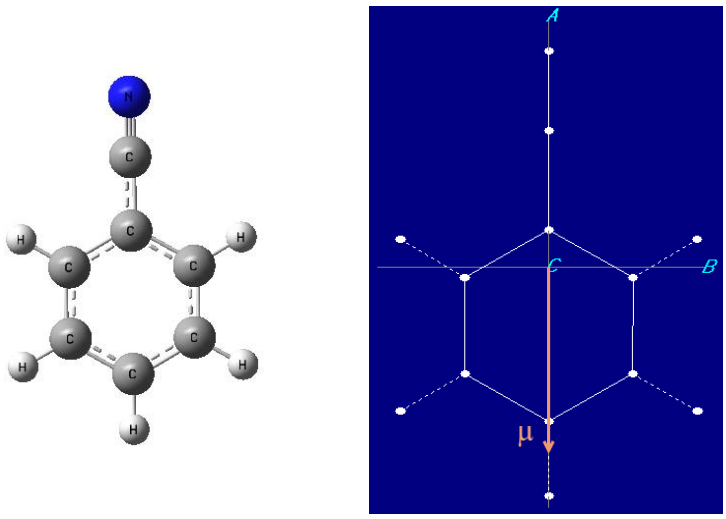


Figure 3.1: Molecular structure and principal axis system of BN

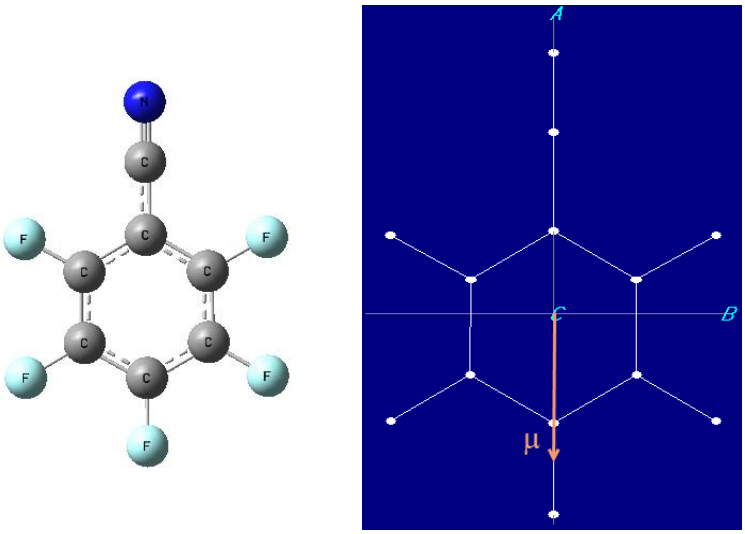


Figure 3.2: Molecular structure and principal axis system of PFBN

According to the molecular structures of BN and PFBN, there are five unique ^{13}C and one ^{15}N isotopologues for these molecules which all show weak *a*-type transitions in the MW spectrum due to the small natural abundance of the ^{13}C (1%) and ^{15}N (0.4%) isotopically substituted species.

The first microwave study on benzonitrile (BN) was reported in 1954 from the simultaneous work of Erlandson [2] and Lide [3] from which the approximate values of the rotational constants were determined for the parent molecule. Afterwards, the MW spectra of BN and its nine minor isotopologues were investigated to evaluate the substitution (r_s) structure [4,5]. Later on, by development of Fourier Transform Microwave (FTMW) spectroscopy, the rotational spectrum of BN was reinvestigated to study the hyperfine structure and to obtain the nuclear quadrupole coupling constant of the ^{14}N nucleus [6,7]. In the meantime, the range of measured rotational transitions was extended to very high J levels which allowed researchers to accurately determine the centrifugal distortion constants [8]. Later on, the high resolution MW spectra of the parent BN and its minor isotopic species were recorded to

obtain a more precise substitution (r_s) structure [9]. The last MW study on BN was reported in 2007 in which the FTMW technique was used to obtain the precise values of dipole moment and the nuclear quadrupole coupling constants [1].

To date, although the rotational spectra of the parent BN and its minor isotopologues are known, the spectroscopic constants of the ^{13}C and ^{15}N isotopic species, apart from the rotational constants (i.e. the centrifugal distortion parameters and the nuclear quadrupole coupling constants) have not been reported. Further, within the experimental structures, only the substitution (r_s) structure has been evaluated for this molecule. In this thesis work however, the range of high resolution spectral measurements for the parent BN and its isotopologues was extended from 4 to 26 GHz region and many new transitions were collected which allowed the precise determination of all the spectroscopic constants for the parent BN and its minor isotopic species. Eventually, the newly evaluated effective (r_0) structure was reported for this molecule.

The rotational spectrum of PFBN was first investigated by Sharma and Doraiswamy in 1968 using a Stark modulated MW spectrometer in the frequency range of 18 to 26 GHz from which the approximate values of rotational constants for the parent PFBN were evaluated [10]. Afterwards in 1992, PFBN was studied by the FTMW technique in the 7 to 11 GHz region from which the values of rotational constants and quadrupole coupling constants were reported for the parent PFBN [11].

From the previous works on PFBN, although the rotational spectrum of the parent molecule is known, the centrifugal distortion parameters have not been determined. Further, the rotational spectra of the minor isotopic species of PFBN, which are vital to derive the experimental structures, have not been investigated in either previous study. In this work, the range of high resolution measurements for the parent PFBN was extended from 4 to 26 GHz

and many new transitions were recorded from which the precise values of all the spectroscopic constants for the parent PFBN were evaluated. In addition to the parent species, the MW spectra of the ^{13}C and ^{15}N isotopologues were investigated and their corresponding spectroscopic constants were reported for the first time. Finally, the newly derived substitution (r_s) and effective (r_0) structures were evaluated.

3-2 Experimental details

The pure samples of BN (99%) and PFBN (99%) were purchased from Sigma-Aldrich. 2 bars of the carrier gas (neon for BN and argon for PFBN) was introduced into a bubbler containing the liquid sample. For BN, the pure rotational spectra of the parent and six minor isotopic species were collected between 4 to 26 GHz using the FTMW instrument which is capable of resolving the nuclear quadrupole hyperfine structure of ^{14}N nucleus. For PFBN, the high resolution MW spectrum of the parent species was reinvestigated using the FTMW instrument between 4 to 26 GHz. For the minor isotopic species, since there were no previous MW studies to date, some broadband MW spectra were recorded using the cp-FTMW instrument to initially assign the weak transitions due to the minor isotopologues and then the corresponding high resolution MW spectra were recorded with the FTMW instrument in the 4 to 26 GHz region.

3-3 Spectral assignment and fitting

The BN spectrum showed strong *a*-type transitions and a sample high resolution spectrum of the parent species is shown in Figure 3.3. A number of 51 *a*-type transitions (and their hyperfine components) were measured for the parent BN spanning J=2 to J=9 and no less

than 11 *a*-type transitions (and their hyperfine components) for each minor isotopic species were collected and then fitted to obtain the corresponding spectroscopic constants which are illustrated in Table 3.1. The observed rotational transitions are provided in Appendix I.

The MW spectrum of PFBN included strong *a*-type transitions and a sample spectrum from the FTMW instrument is illustrated in Figure 3.4. A survey broadband MW spectrum from the cp-FTMW instrument is also shown in Figure 3.5 in which the weak transitions due to some of the ^{13}C isotopologues are shown. A number of 251 *a*-type transitions (and their hyperfine components) for the parent PFBN between 4 to 26 GHz (J=4 to 23) and a minimum of 26 *a*-type transitions (and their hyperfine components) for the minor isotopic species were measured. The fitted spectroscopic constants are filled in Table 3.2 and the measured rotational transitions are listed in Appendix II.

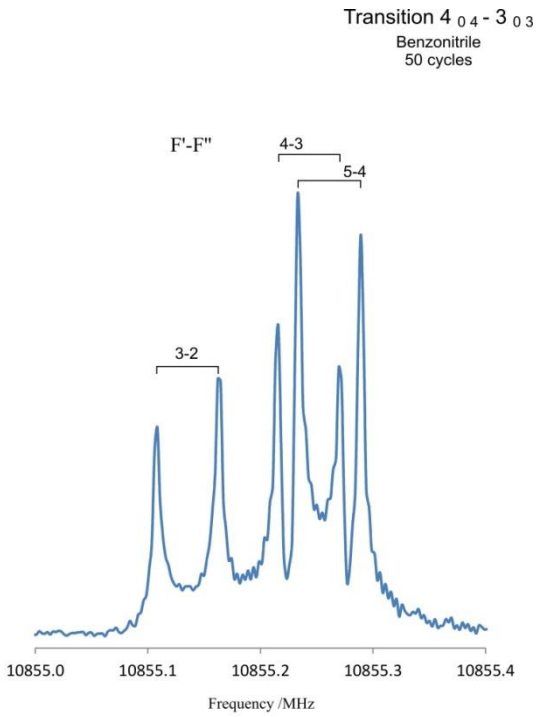


Figure 3.3: Sample FTMW spectrum of the 4 $_{0\ 4}$ - 3 $_{0\ 3}$ rotational transition of BN showing the hyperfine splitting arising from the ^{14}N quadrupolar nucleus

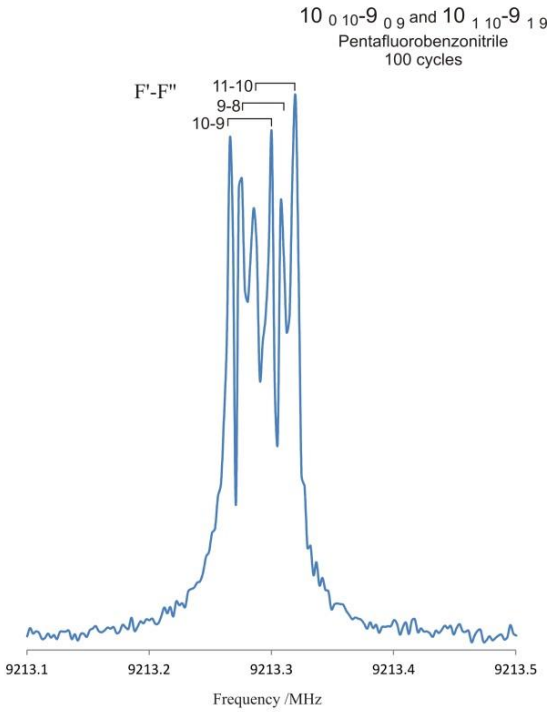


Figure 3.4: Sample FTMW spectrum of the $10_{0\,10} - 9_{0\,9}$ and $10_{1\,10} - 9_{1\,9}$ rotational transitions of PFBN showing the hyperfine splitting arising from the ^{14}N quadrupolar nucleus

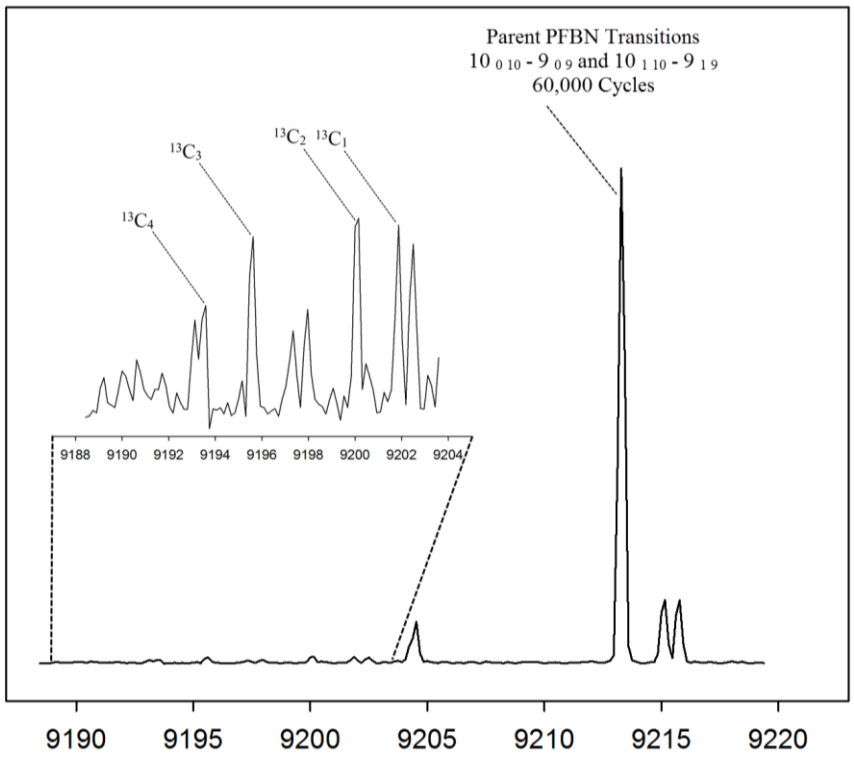


Figure 3.5: Sample cp-FTMW spectrum of PFBN showing $10_{0\,10} - 9_{0\,9}$ and $10_{1\,10} - 9_{1\,9}$ rotational transitions for the parent and some of the minor isotopologues

Table 3.1: Spectroscopic constants of BN and its minor isotopic species

	Normal	$^{13}C_1$	$^{13}C_2$	$^{13}C_3$	$^{13}C_4$	$^{13}C_5$	^{15}N
Rotational Constants /MHz							
A	5655.2654(22)	5655.5075(55)	5563.9185(45)	5565.6669(50)	5655.4544(75)	5655.2407(31)	5655.270(15)
B	1546.875786(64)	1545.55183(16)	1546.80340(13)	1535.71304(14)	1523.65523(16)	1528.64068(16)	1502.14915(29)
C	1214.404054(55)	1213.60145(10)	1210.089719(98)	1203.37302(10)	1200.05780(10)	1203.136829(95)	1186.65856(21)
Centrifugal Distortion Constants /kHz							
Δ_J	0.04503(34)	0.04616(77)	0.04572(64)	0.04509(69)	0.0446(10)	0.04512(86)	0.0392(37)
Δ_{JK}	0.9373(19)	0.879(18)	0.921(13)	0.937(14)	0.907(26)	0.899(21)	0.911(28)
δ_J	0.01119(23)	0.01110(72)	0.01146(64)	0.01103(70)	0.01186(77)	0.01057(74)	0.0172(38)
δ_K	0.603(13)	0.603	0.603	0.603	0.603	0.603	0.603
^{14}N Nuclear Quadrupole Coupling Constants /MHz							
$1.5\chi_{aa}$	-6.35600(83)	-6.3438(84)	-6.3666(80)	-6.3661(86)	-6.345(14)	-6.360(16)	N/A
$0.25(\chi_{bb}-\chi_{cc})$	0.08483(34)	0.0724(51)	0.0696(48)	0.0681(52)	0.0749(48)	0.0758(53)	N/A
rms /kHz	0.95	1.03	1.06	1.15	0.90	0.99	0.39
no. lines	177	51	63	63	42	39	11

Table 3.2: Spectroscopic constants of PFBN and its minor isotopic species

	Normal	$^{13}C_1$	$^{13}C_2$	$^{13}C_3$	$^{13}C_4$	$^{13}C_5$	^{15}N
Rotational Constants /MHz							
A	1029.368635(32)	1029.40041(35)	1026.38602(26)	1026.36077(29)	1029.40457(34)	1029.36990(42)	1029.3708(25)
B	764.5952880(91)	762.92535(24)	764.329754(66)	763.68961(11)	761.72244(24)	756.63541(27)	748.4102(14)
C	438.7218484(60)	438.177629(29)	438.092228(27)	437.877120(26)	437.781250(31)	436.089678(33)	433.343572(41)
Centrifugal Distortion Constants /kHz							
Δ_J	0.006169(18)	0.006096(92)	0.006199(85)	0.006150(84)	0.006262(96)	0.00616(10)	0.00613(12)
Δ_{JK}	0.044977(74)	0.0478(23)	0.0454(16)	0.0468(16)	0.0463(19)	0.0453(27)	0.0429(26)
Δ_K	-0.02835(34)	-0.02835	-0.02835	-0.02835	-0.02835	-0.02835	-0.02835
δ_J	0.0023687(96)	0.0023687	0.0023687	0.0023687	0.0023687	0.0023687	0.0023687
δ_K	0.029550(65)	0.029550	0.029550	0.029550	0.029550	0.029550	0.029550
^{14}N Nuclear Quadrupole Coupling Constants /MHz							
$1.5\chi_{aa}$	-6.5807(12)	-6.583(39)	-6.574(20)	-6.577(23)	-6.592(39)	-6.625(45)	N/A
$0.25(\chi_{bb}-\chi_{cc})$	0.10804(68)	0.1055(29)	0.1107(26)	0.1082(26)	0.1080(29)	0.1080(34)	N/A
rms /kHz	0.79	1.19	1.18	1.16	1.18	1.36	0.64
no. lines	753	81	99	96	81	78	30

Comparing data in Table 3.1 and Table 3.2 shows that the number of measured lines for PFBN (251 transitions, 753 hyperfine lines) is much more than that of BN (51 transitions, 177 hyperfine lines). In addition, the measured transitions for PFBN cover higher rotational energy levels up to J=23 whereas those of BN span up to J=9. Therefore, one can say that at the very cold temperatures of supersonic jet, there are more available rotational energy levels for PFBN compared to BN. This is due to the fact that PFBN is a heavier molecule than BN and it has larger moments of inertia and smaller rotational constants. This results in shifting the population distribution of molecules towards the higher rotational energy levels for the heavier PFBN relative to BN.

From Table 3.1 and Table 3.2 it can also be seen that for both BN and PFBN, the values of rotational constants for the minor isotopic species slightly differ (by few MHz) from those of the parent molecule which is due to the change in their moments of inertia and principal axes with heavy atom substitution. Further, the centrifugal distortion constants for both BN and PFBN have non-zero values, which confirms the fact that real molecules are not rigid. The smaller magnitude of centrifugal distortion parameters for PFBN compared to BN reveals that the PFBN molecule has a more rigid molecular structure. From Table 3.1 and Table 3.2 it is also found that the spectral fitting for the parent BN was not responsive to the Δ_K centrifugal constant as this constant was found to be strongly correlated to the A rotational constant. Hence, the Δ_K parameter was removed from the least-squares spectral fit. Further, for the minor isotopic species of BN, the δ_K parameter was fixed at the value of the parent molecule as it could not be determined precisely due to the lack of transitions with the high K_a values for the isotopologues. For PFBN however, all the quartic centrifugal distortion constants for the parent molecule could be precisely determined while most of the centrifugal distortion parameters of the isotopic species (i.e. Δ_K, δ_J and δ_K parameters) were fixed at the

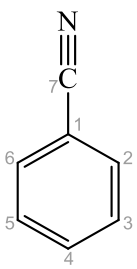
values of the parent PFBN similarly because of the small number of transitions observed for the minor isotopologues.

For both BN and PFBN, the ^{14}N nuclear quadrupole coupling constants for the minor ^{13}C isotopologues show a small degree of variation (within few kHz) compared to those of the parent molecule, because the principal axes of the molecule slightly change by the heavy ^{13}C substitution. Such close values of the quadrupole coupling constants is not surprising as the electronic environment surrounding the nitrogen atom does not change that much by heavy atom substitution.

3-4 Structural determination

The value of inertial defect $\Delta_0 = I_c - I_b - I_a$, which is a measure of the deviation from the planarity, has a non-zero (though small) value of 0.080 amu.Å^2 for BN and 0.001 amu.Å^2 for PFBN, as expected for planar molecules. Assuming planarity, the ground state rotational constants of the parent BN and PFBN and their minor isotopologues were used to obtain the substitution (r_s) and effective (r_0) structures for these two molecules. The equilibrium (r_e) geometries were also calculated at MP2/6-311++G(2d,2p) level of theory. The experimental (r_s and r_0) and theoretical (r_e) structures of BN and PFBN are shown in Table 3.3 and Table 3.4, respectively.

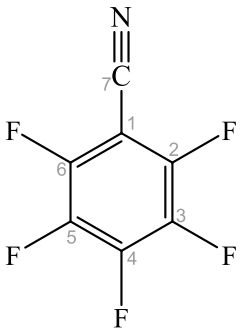
Table 3.3: The substitution (r_s), effective (r_0) and *ab initio* (r_e) structures of BN (bond lengths in Ångstrom and bond angles in degrees)



Structural Parameter	r_s	r_0	r_e^*
C1–C2	1.381(6)	1.397(2)	1.401
C2–C3	1.415(12)	1.395(2)	1.393
C3–C4	1.396(1)	1.397(1)	1.396
C1–C7	1.450(3)	1.445(3)	1.435
C7–N	1.158(1)	1.158(1)	1.173
∠(C1–C2–C3)	118.1(4)	119.1(2)	119.5
∠(C2–C3–C4)	120.2(1)	120.1(3)	120.3
∠(C3–C4–C5)	120.1(1)	120.2(1)	120.0
∠(C6–C1–C2)	123.2(6)	121.3(3)	120.5
∠(C7–C1–C2)	118.4(4)	119.4(2)	119.8

* Calculated at MP2/6-311++G(2d,2p) level

Table 3.4: The substitution (r_s), effective (r_0) and *ab initio* (r_e) structures of PFBN (bond lengths in Ångstrom and bond angles in degrees)



Structural Parameter	r_s	r_0	r_e^*
C1–C2	1.400(2)	1.392(2)	1.398
C2–C3	1.360(3)	1.382(2)	1.388
C3–C4	1.391(1)	1.390(1)	1.392
C1–C7	1.436(1)	1.437(3)	1.426
C7–N	1.157(1)	1.156(1)	1.173
∠(C1–C2–C3)	121.6(2)	121.0(2)	120.9
∠(C2–C3–C4)	119.8(1)	119.6(2)	119.6
∠(C3–C4–C5)	119.8(1)	120.2(2)	120.4
∠(C6–C1–C2)	117.4(2)	118.6(2)	118.6
∠(C7–C1–C2)	121.3(1)	120.7(1)	120.7

* Calculated at MP2/6-311++G(2d,2p) level

It can be found from Table 3.3 that the substitution structure for BN (the r_s column) is not well determined as some structural parameters contain large Costain errors, e.g. C1–C2 and C2–C3 distances and C6–C1–C2 angle. In contrast, the substitution structure for PFBN (the r_s column in Table 3.4) is better determined as the largest uncertainty in bond length values is only 0.003 Å and that in bond angles is just 0.2°.

The reason for the larger uncertainties in the r_s structural parameters for BN compared to that for PFBN can be found by looking at the principal axis systems of both molecules in Figure 3.6 in which the origin of the axis system is the center of mass of the molecule.

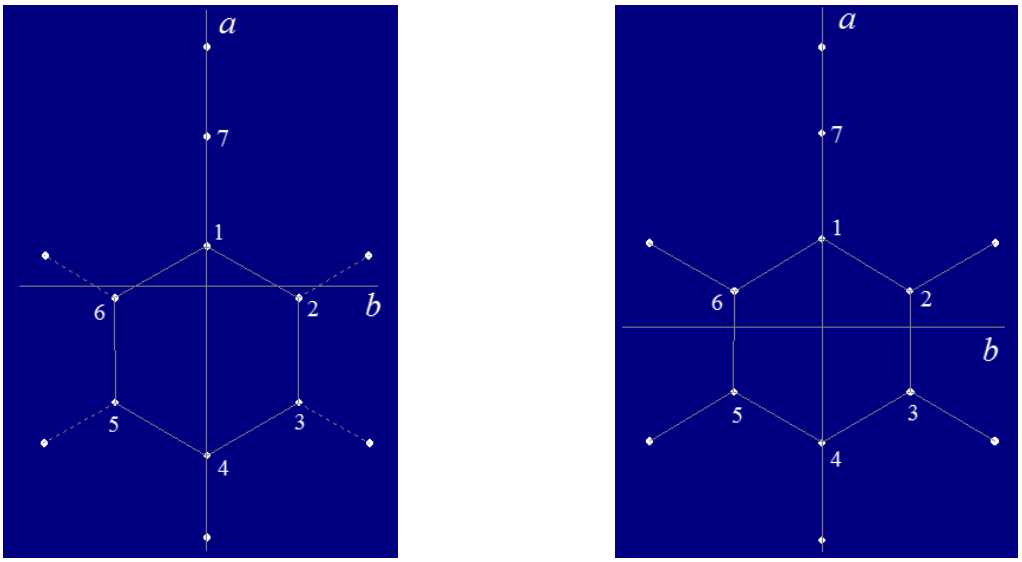


Figure 3.6: Comparison of the principal axis systems of BN (left) and PFBN (right)

In PFBN, the center of mass is close to the center of the ring and all the atoms are far away from the center of mass and there is no atom close to the principal inertial axes *a* or *b*. However, the center of mass in BN is shifted towards the cyano group which causes C2 and C6 atoms to be close to the *b* principal axis and therefore to have small *a* coordinates for these two atoms.

In a Kraitchman analysis, the uncertainty in a coordinate is calculated by Costain's rule in which the uncertainty is inversely related to the absolute value of the coordinate, dz=0.0015/|z| [12]. Based on the Costain's rule, the small *a* coordinate for the C2 and C6 atoms causes a large uncertainty in the *a* coordinate for these two atoms and that is the reason that the r_s structural parameters involving C2 and C6 atoms, e.g. C1–C2 and C2–C3 distances and C6–C1–C2 angle, are not reliably determined. In fact, the issue of the presence of atoms with the small coordinates and its effect on the r_s structure was also observed while studying the related aromatic compounds including fluorobenzene in which the C2 and C6 atoms suffer from the small *a* coordinate and an inaccurate substitution structure is derived for this molecule [13-14].

The effective (r_0) structures of BN and PFBN are also shown in Table 3.3 and Table 3.4. The r_0 structures for both molecules are well determined as the uncertainties in bond lengths do not exceed 0.003 Å and those in bond angles do not go beyond 0.3°. For BN, which suffers from the large uncertainties in the most r_s structural parameters, the r_0 structure is a clear improvement in its structural determination which arises from using the least-squares approach. It is worth mentioning that to improve the r_0 fit for BN, only two rotational constants A and B (instead of three A, B and C constants) for each isotopic species, which means a total of 14 experimentally determined A and B rotational constants for the parent and isotopologues, were used in the fit. Using only A and B rotational constants, compared to

other linear combinations of rotational constants, gave a more satisfactory structural fit for BN.

3-5 Discussion

In the current study, BN is considered to be the reference compound and its geometry changes upon fluorination were studied. For the sake of comparisons in this chapter, the r_0 and r_e structures of BN and PFBN are used while the r_s structures will not be utilized as the r_s structure for BN, which is the reference compound, could not be reliably determined.

It is worthwhile to first examine the structure of BN itself to find out how the cyano group distorts the perfect hexagonal benzene ring with angles of 120°. According to the r_0 structure of BN, the angle at the substituted carbon (C1), i.e. the C6–C1–C2 angle, widens by 1.3° while the adjacent angles at C2 or C6 contract by 0.9°. The rest of the angles at C3, C4 and C5 are barely affected relative to benzene. The revealed structural changes based on the r_0 parameters are in good agreement with the trends observed from the MP2 theory predictions although the *ab initio* values for the changes of angles at C1 and C2 are less drastic. All in all, it is found that the most structural deformations in BN happen around the cyano substituted carbon (C1) and fewer distortions are observed by going far away from C1.

To realize the effect of full fluorination on the geometry of BN, a comparison between PFBN and BN is made based on the r_0 and r_e structures. This comparison is shown in Figure 3.7 in which the structural changes are calculated by considering BN as the reference compound. Any positive change indicates an increase in the structural parameter (increase of bond length or bond angle) whereas a negative variation shows the reduction of the structural parameter (contraction of bond length or bond angle) relative to BN.

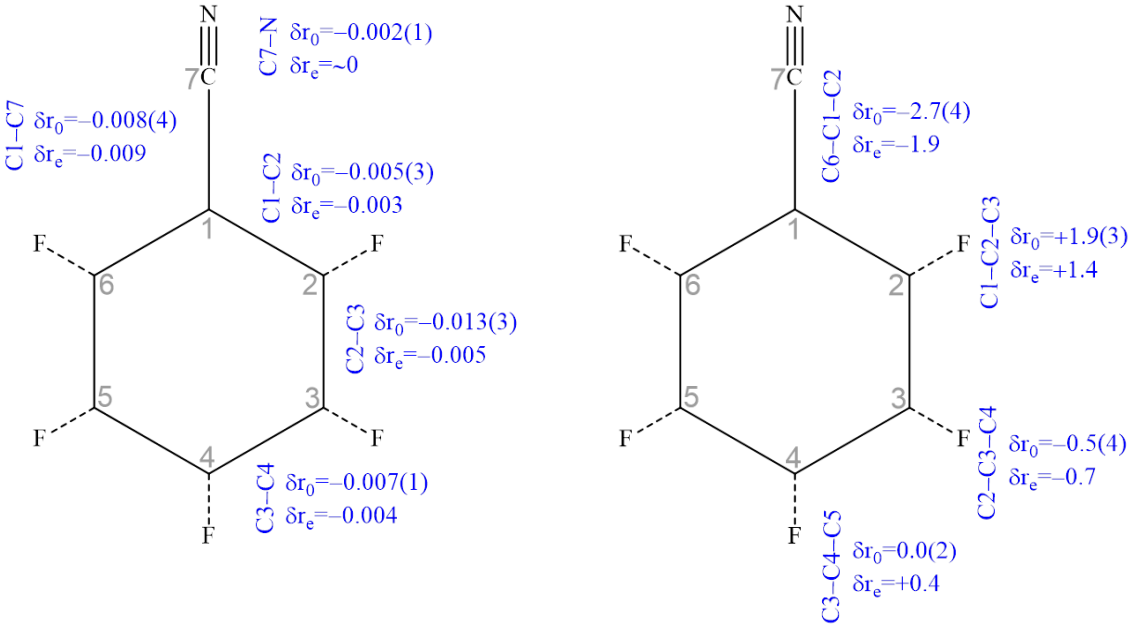


Figure 3.7: Structural changes in PFBN as a function of full fluorination based on r_0 and r_e structures and by considering BN as the reference compound. Bond length and bond angle differences are in Ångstroms and degrees, respectively.

First, the variation of bond lengths in PFBN is examined; Based on the δr_0 values it at can be seen that all the bonds in the ring are shortened and the most distorted distance is C2–C3 (and also C5–C6) which is shortened by 0.013 Å. The outer ring bond C1–C7 undergoes a shortening of 0.008 Å as well while the C7–N distance remains almost unaffected. Similar changes in the bond lengths are predicted by the MP2 theory (δr_e values).

Regarding the ring bond angles and according to the δr_0 values, the most affected angle is C6–C1–C2 which is reduced by 2.7° and then the neighboring angles at C2 and C6 which are opened by 1.9°. There are minimal changes for the rest of ring bond angles at C3, C4 and C5. Similar structural changes are seen from the δr_e values.

All in all and according to the δr_0 and δr_e values, one can say that the most structural deformations in PFBN happen around the cyano substituted carbon (C1) and minimal distortions are seen in the opposite part of the ring to the cyano group.

The observed distortions upon full fluorination in PFBN can be explained by examining the distortions in related fluorinated aromatic compounds, e.g. fluorinated benzenes [15]. Single site fluorination of benzene deforms the ring backbone and causes an expansion of the C–C–C angle at the fluorination site by few degrees (2–3°), contraction of the adjacent angles by few degrees and shortening of the neighbouring C–C bonds [15]. These ring distortions can be interpreted by Bent's rule which is based on a distorted hybridization model and states that "atomic *s* character tends to concentrate in orbitals that are directed toward electropositive groups and atomic *p* character tends to concentrate in orbitals that are directed toward electronegative groups" [16]. According to the Bent's rule, the σ-bonding hybrid orbital of the C–F bond holds more *p* character while the other two hybrid orbitals of the carbon, which form the adjacent C–C bonds, maintain less *p* character (more *s* character) which causes two effects: 1) widening of the angle at the fluorination site and 2) shortening of the neighbouring C–C bonds [17-18].

The distortion of carbon's hybridization at the fluorination sites was confirmed by the results of a natural bonding orbital (NBO) analysis performed at the MP2/6-311++G(2d,2p) level of theory and is schematically shown in Figure 3.8. The numbers on BN hybridization scheme show the percentage of the *s* and *p* characters of the carbon atoms' hybrid orbitals (an idealized sp^2 hybrid has 33% *s* characters and 67% *p* character) and the numbers on the PFBN hybridization scheme indicate the change in the *s* or *p* characters upon fluorination at different sites. As it can be seen from Figure 3.8, in PFBN, there are five fluorine atoms substituted in proximity which all compete for the attraction of the *p* character (by 5%) from the hybrid orbitals of the C−F bonds towards them [15] and consequently there will be more *s* character (by 1 to 4%) in the carbon valences in the ring towards the adjacent carbons which leads to shorter C−C bonds.

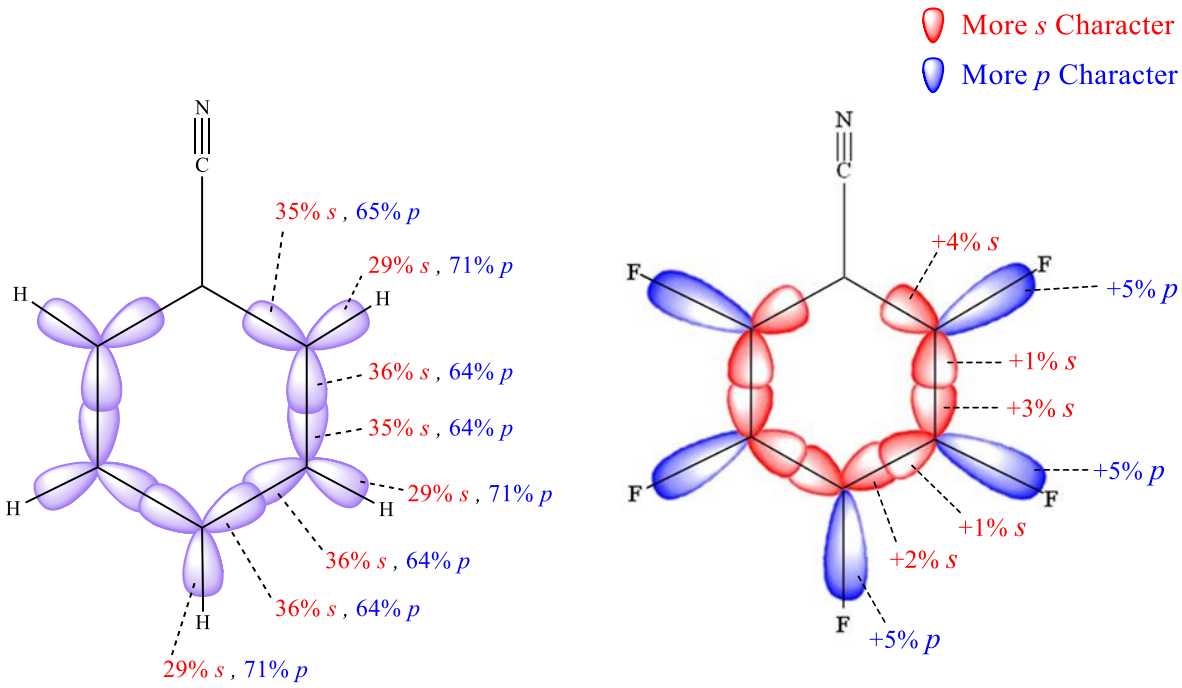


Figure 3.8: The composition of carbons' hybrid orbitals in BN (left) and perturbation of hybridization in PFBN caused by full fluorination (right) according to the NBO analysis results

This justifies the fact that all the ring bonds in PFBN are shortened and the whole ring is more compact than in BN. The C7–N bond seems to remain unaffected by the full fluorination which is not surprising as the fluorine atoms cannot extend their inductive effects far from their vicinities.

When it comes to interpretation of the bond angle changes in PFBN, it should be noticed that all fluorine atoms in PFBN tend to increase the angle at their substitution sites which is not possible in practice because if one of the ring bond angles is widened, the neighboring angles must usually contract to compensate for that change [19]. Nevertheless, examining the hybridization at different ring sites in PFBN explains why the most angular deformations happen around C1 and less distortions are seen by going far away from C1. In fact, the hybridization at the fluorination sites, i.e. at C2, C3, C4, C5 and C6, is mostly disturbed due to the high electronegativity of fluorine atom whereas the hybridization at C1 is not much

affected due to the lower electronegativity of the cyano group compared to fluorine. As a result, the angle at C1 can be more easily decreased due to the induction effect of the two fluorine atoms at C2 and C6 and the angles at C2 and C6 are opened to compensate. The rest of the angles at C3, C4 and C5 cannot be drastically deformed as there are no carbon atoms in their vicinities with unperturbed hybridization. In other words, the vicinity of C1 in PFBN is more flexible in terms of angular distortions.

In summary to this chapter, the results of the MW studies for BN and PFBN were presented and the experimental (r_s and r_0) and theoretical (r_e) structures for both molecules were evaluated. It was found that the substitution (r_s) structure for BN could not be reliably determined as there were some atoms in the molecule with fairly small coordinates. A comparison between BN and PFBN was then made based on the r_0 and r_e structures and by considering BN as the reference compound. From that comparison, it was found that the full fluorination of BN will result in clear distortions in the geometry of BN. The structural changes based on the r_0 structures, which were supported by the *ab initio* predictions, showed that most geometrical distortions in PFBN happen around the cyano substituted carbon and fewer distortions are seen by going far away from that point. Eventually, the structural deformations as a function of full fluorination were interpreted by the hybridization theory.

In Chapter 4, the results of MW studies and structural determination for two of the mono-fluorinated derivatives of BN including 2-fluorobenzonitrile (2FBN) and 3-fluorobenzonitrile (3FBN) will be presented. In addition, the effect of single fluorine substitution at the *ortho* and *para* positions on the geometry of BN will be discussed.

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Chapter 4: Microwave study and molecular structure of 2-fluorobenzonitrile and 3-fluorobenzonitrile

To realize the effect of single fluorination on the geometry of benzonitrile, two mono-fluorinated derivatives of benzonitrile were studied and chosen to be 2-fluorobenzonitrile (2FBN) and 3-fluorobenzonitrile (3FBN). In this chapter, the results of the MW studies and structural determination for 2FBN and 3FBN are presented and the effect of single fluorination at the *ortho* and *meta* positions on the geometry of benzonitrile is described.

4-1 Introduction

The molecular structures of 2FBN and 3FBN and their principal axis systems are illustrated in Figure 4.1 and Figure 4.2. Both molecules are planar with no rotational symmetry axis and therefore have the point group of C_s. The total dipole moment of 2FBN is estimated to be 6.03 D [at MP2/6-311++G(2d,2p) level] with components of μ_A = 5.97 D and μ_B = 0.81 D and therefore, strong *a*-type and weaker *b*-type rotational transitions are expected for 2FBN. For 3FBN, the total dipole moment value is calculated to be 4.34 D at the same level of theory with the components of μ_A = 3.45 D and μ_B = 2.64 D and hence strong *a*- and *b*-type rotational transitions are expected for 2FBN.

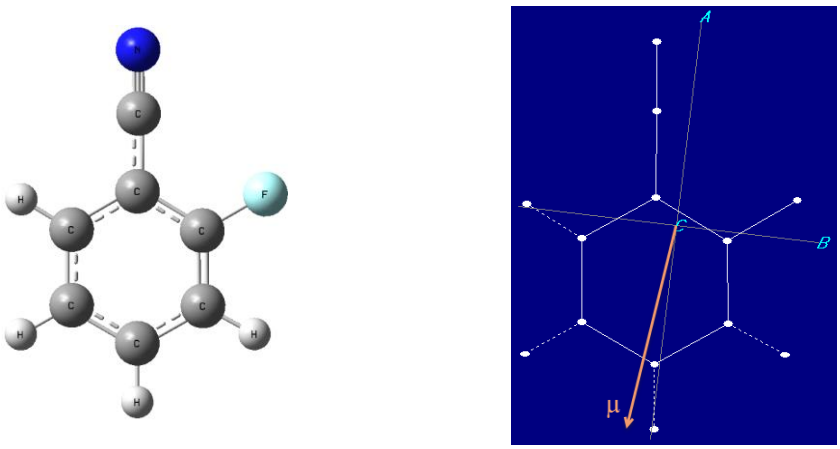


Figure 4.1: Molecular structure and principal axis system of 2FBN

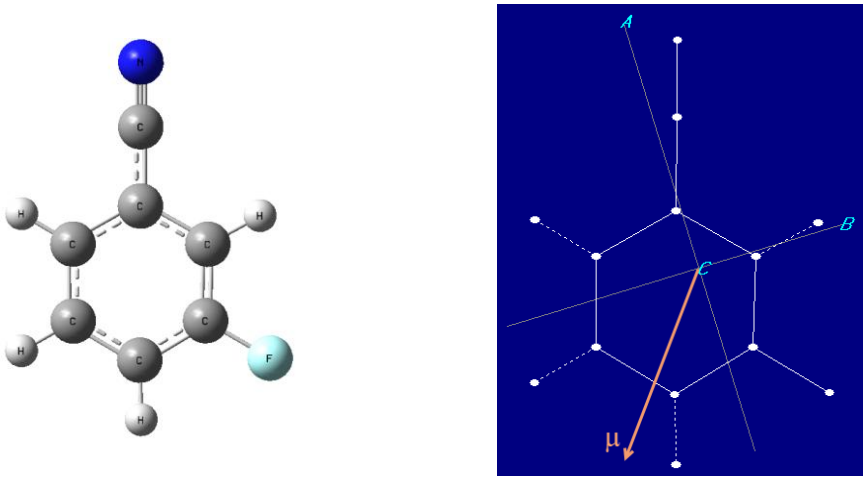


Figure 4.2: Molecular structure and principal axis system of 3FBN

From the molecular structures of 2FBN and 3FBN, since all carbon atoms are in different chemical environments within the molecule, there will be seven unique ^{13}C isotopic species as well as one ^{15}N minor isotopic species for these molecules. All the minor isotopologues show weak rotational transitions in the MW spectrum due to the small natural abundance of ^{13}C and ^{15}N substituted species.

The first MW study on 2FBN was conducted by Bottcher and Sutter in 1986 in which the FTMW technique was used to determine the rotational constants, centrifugal distortion parameters and the nuclear quadrupole coupling constants of the parent species [1]. However, due to the lack of assignments of the rotational transitions belonging to high J and K_a values, the centrifugal distortion constants were not accurately determined in that work. Afterwards, the rotational spectrum of 2FBN was reinvestigated by Dutta et al. in 1987 using a Stark modulated MW technique from which the rotational constants of the parent 2FBN were measured and an approximate r_0 structure was evaluated based on the reproduction of the observed principal moments of inertia of the parent species determined from the low resolution spectra [2]. Eventually in 2006, from the work of Varadwaj et al., the range of

collected rotational transitions was extended to the millimetre-wave region and more precise values of centrifugal distortion constants for the parent 2FBN were evaluated [3].

In the previous works on 2FBN, although there have been some MW studies on the parent molecule, the MW spectra of the minor isotopic species of 2FBN, which are vital to evaluate the accurate experimental structure, were not investigated. In this work, however, the MW spectrum of the parent 2FBN was reinvestigated in which the range of high resolution spectral measurements was extended from 4 to 26 GHz and many new transitions were collected which allowed the precise determination of spectroscopic constants of the parent 2FBN including the rotational constants, centrifugal distortion parameters and the nuclear quadrupole coupling constants. Further, the high resolution MW spectra of the ^{13}C and ^{15}N isotopologues of 2FBN were studied for the first time and the newly evaluated substitution (r_s) and effective (r_0) structures were reported.

The rotational spectrum of 3FBN was first investigated by the low resolution MW study of Dutta et al. in 1986 [4]. From that work, the approximate values of rotational constants and centrifugal distortion parameters of the parent species were determined and an approximate r_0 structure was proposed based on the reproduction of the rotational constants of the parent species. Later on in 1987, the FTMW technique was used to probe the nuclear quadrupole hyperfine structure of the rotational spectrum and to obtain more precise values of the rotational constants and the centrifugal distortion parameters for the parent 3FBN [5].

To date, although the MW spectrum of the parent 3FBN is known, there have been no MW studies on the minor isotopic species of 3FBN which are required to derive the accurate experimental structure. In this work, the rotational spectrum of the parent 3FBN was reinvestigated and the range of high resolution MW measurements was extended from 4 to 26 GHz and many new transitions were measured and included in the fit to obtain the accurate

values for all of the spectroscopic constants of the parent species. In addition, the high resolution MW spectra of the minor ^{13}C and ^{15}N isotopic species were investigated for the first time which allowed the evaluation of the substitution (r_s) and effective (r_0) structures.

4-2 Experimental details

The pure samples of 2FBN (98%) and 3FBN (98%) were purchased from Sigma-Aldrich. 2 bars of the carrier gas (argon) was introduced into a bubbler containing the liquid sample. Although the boiling points of these compounds are high, 90 °C for 2FBN (at 21 mmHg) and 182°C for 3FBN (at 753 mmHg), the generated vapor pressure was sufficient to give a strong S/N ratio, mainly due to the large dipole moments of these two molecules. For both 2FBN and 3FBN, the pure rotational spectrum of the parent species was reinvestigated using the FTMW instrument between 4 to 26 GHz in which some rotational transitions were re-measured and many new transitions were collected. In addition to the parent 2FBN and 3FBN, the high resolution MW spectra of the ^{13}C and ^{15}N isotopologues were measured with the FTMW instrument in the same region.

4-3 Spectral assignment and fitting

The spectrum of 2FBN showed strong *a*-type and weaker *b*-type transitions as predicted from the calculated values of dipole moment components (μ_A = 5.97 D and μ_B = 0.81 D). A sample high resolution MW spectrum for the parent 2FBN is demonstrated in Figure 4.3 in which the hyperfine splitting in the rotational spectrum is due to the ^{14}N quadrupolar nucleus. A number of 88 *a*-type and 27 *b*-type transitions (and their hyperfine components) were measured for the parent 2FBN spanning J = 2 to J = 12 and no less than 12 *a*-type transitions (and their hyperfine components) were collected for the isotopologues. It is worth mentioning that for

the 2FBN minor isotopologues, the *b*-type transitions were not observed as the μ_B dipole component and the natural abundance of these isotopes are small. By fitting the measured rotational transitions to the Watson's A-reduced Hamiltonian (I^r representation), the spectroscopic constants of the parent 2FBN and its minor isotopic species were evaluated which are illustrated in Table 4.1. The observed rotational transitions are provided in Appendix III.

The MW spectrum of 3FBN included strong *a*-type and *b*-type transitions which arose from the large values of dipole moment components (μ_A = 3.45 D and μ_B = 2.64 D). A sample spectrum from the FTMW instrument for the parent 3FBN is demonstrated in Figure 4.4. A total of 72 *a*-type and 75 *b*-type transitions (and their hyperfine components) were measured for the parent 3FBN spanning J = 2 to J = 13 and a minimum of 10 *a*-type and 4 *b*-type transitions were collected for the minor isotopic species. It has to be mentioned that for the minor isotopic species of 3FBN, both *a*-type and *b*-type transitions were observable because of the considerable values of dipole moment components μ_A and μ_B. The obtained spectroscopic constants from fitting the measured rotational spectra to the same Hamiltonian as for 2FBN, are shown in Table 4.2. A list of measured rotational transitions is provided in Appendix IV.

According to Table 4.1 and 4.2, it is found that while the extent of variation in the rotational constants for each parent species and minor isotopologues is within few MHz, the quadrupole coupling constants are minimally changed (by few kHz) as the electronic environment around the nitrogen atom remains almost unaffected by heavy atom substitution. From these tables it can also be seen that the centrifugal distortion constants for both 2FBN and 3FBN have non-zero values which reveals these molecules are not rigid rotors.

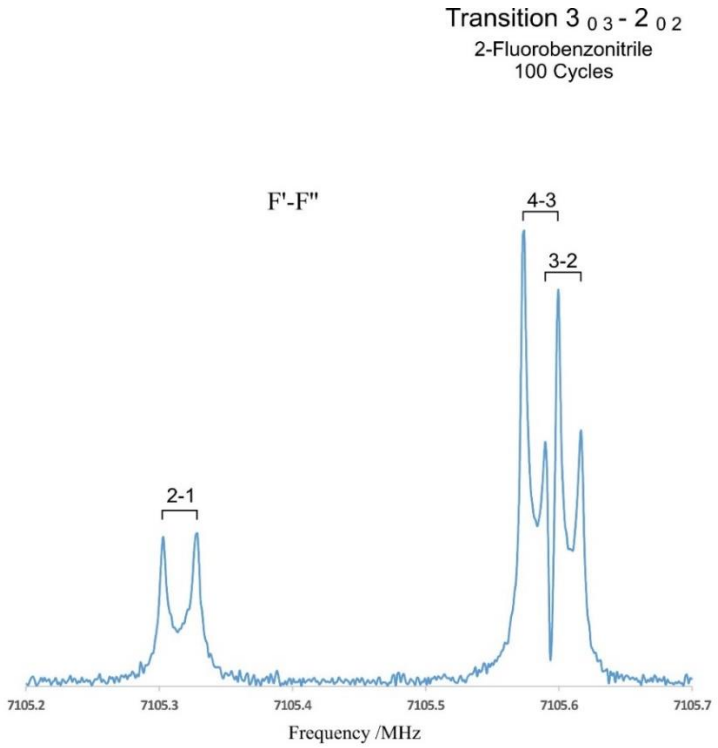


Figure 4.3: Sample FTMW spectrum of the 3 $_{0\,3}$ - 2 $_{0\,2}$ rotational transition of 2FBN showing the hyperfine splitting arising from the ^{14}N quadrupolar nucleus

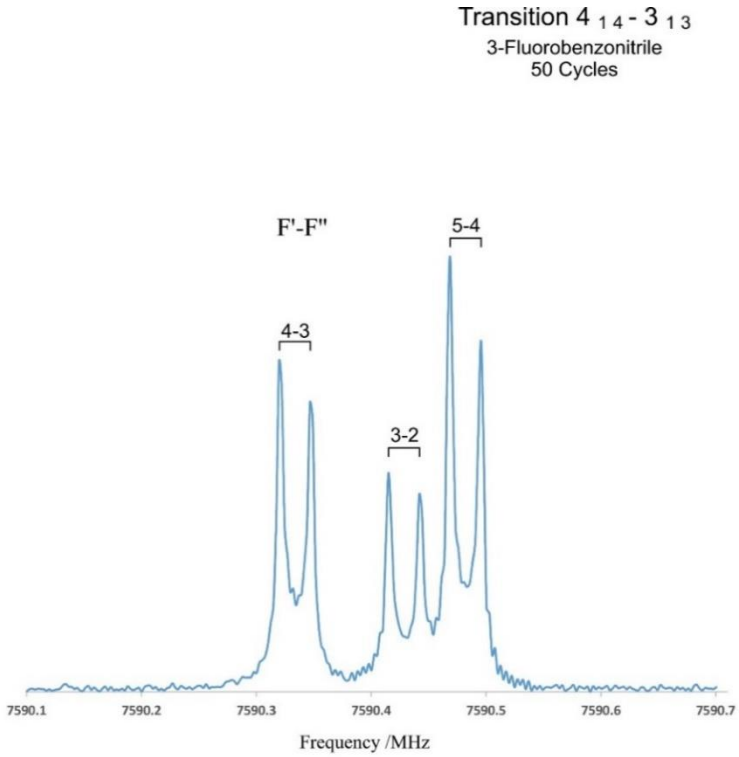


Figure 4.4: Sample FTMW spectrum of the 4 $_{1\,4}$ - 3 $_{1\,3}$ rotational transition of 3FBN showing the hyperfine splitting arising from the ^{14}N quadrupolar nucleus

Table 4.1: Spectroscopic constants of 2FBN and its minor isotopic species

	Normal	$^{13}C_1$	$^{13}C_2$	$^{13}C_3$	$^{13}C_4$	$^{13}C_5$
Rotational Constants /MHz						
A	2940.761152(88)	2938.1093(17)	2928.2765(19)	2922.5544(18)	2940.6938(25)	2910.0201(16)
B	1512.700202(21)	1511.90776(24)	1512.65044(24)	1502.35519(24)	1488.44249(32)	1498.29853(23)
C	998.652009(12)	998.00280(13)	997.18660(15)	992.04534(15)	988.01581(19)	988.82807(13)
Centrifugal Distortion Constants /kHz						
Δ_J	0.04051(15)	0.0416(36)	0.0428(39)	0.0370(37)	0.0404(46)	0.0429(35)
Δ_{JK}	0.50834(79)	0.506(26)	0.519(30)	0.543(28)	0.473(35)	0.477(25)
Δ_K	0.4332(82)	0.4332	0.4332	0.4332	0.4332	0.4332
δ_J	0.012496(79)	0.0135(23)	0.0135(25)	0.0102(24)	0.0122(31)	0.0131(23)
δ_K	0.3018(10)	0.3018	0.3018	0.3018	0.3018	0.3018
^{14}N Nuclear Quadrupole Coupling Constants /MHz						
$1.5\chi_{aa}$	-6.27359(75)	-6.2736(60)	-6.2856(95)	-6.3014(76)	-6.2776(92)	-6.2329(58)
$0.25(\chi_{bb}-\chi_{cc})$	0.06078(20)	0.0572(23)	0.0574(27)	0.0637(27)	0.0604(33)	0.0557(24)
rms /kHz	1.04	0.95	1.01	1.00	1.24	0.91
no. lines	372	43	40	40	40	42

Table 4.1 continued

	$^{13}C_6$	$^{13}C_7$	^{15}N
Rotational Constants /MHz			
A	2901.5869(16)	2935.6537(17)	2932.9825(14)
B	1511.98054(25)	1497.25539(22)	1473.13738(26)
C	993.78335(14)	991.31529(14)	980.37874(14)
Centrifugal Distortion Constants /kHz			
Δ_J	0.0435(39)	0.0414(34)	0.0416(24)
Δ_{JK}	0.477(28)	0.510(26)	0.496(18)
Δ_K	0.4332	0.4332	0.4332
δ_J	0.0128(25)	0.0137(22)	0.0125(19)
δ_K	0.3018	0.3018	0.3018
^{14}N Nuclear Quadrupole Coupling Constants /MHz			
$1.5\chi_{aa}$	-6.2601(63)	-6.2879(61)	N/A
$0.25(\chi_{bb}-\chi_{cc})$	0.0547(24)	0.0618(22)	N/A
rms /kHz	0.99	0.94	0.41
no. lines	42	42	12

Table 4.2: Spectroscopic constants of 3FBN and its minor isotopic species

	Normal	$^{13}C_1$	$^{13}C_2$	$^{13}C_3$	$^{13}C_4$	$^{13}C_5$
Rotational Constants /MHz						
A	3388.610721(63)	3388.57484(74)	3370.8436(13)	3384.43373(66)	3370.32359(75)	3313.22625(80)
B	1186.639029(12)	1184.27282(18)	1186.66485(35)	1181.29819(16)	1178.40377(19)	1185.29439(21)
C	878.6966535(88)	877.397519(81)	877.51383(14)	875.485277(75)	872.951907(86)	872.811559(89)
Centrifugal Distortion Constants /kHz						
Δ_J	0.039199(63)	0.0384(11)	0.0371(20)	0.0399(10)	0.0391(12)	0.0351(13)
Δ_{JK}	0.01075(53)	0.01075	0.01075	0.01075	0.01075	0.01075
Δ_K	1.2574(55)	1.2574	1.2574	1.2574	1.2574	1.2574
δ_J	0.013910(33)	0.01418(92)	0.0121(17)	0.01523(85)	0.01429(97)	0.0109(10)
δ_K	0.18152(86)	0.18152	0.18152	0.18152	0.18152	0.18152
^{14}N Nuclear Quadrupole Coupling Constants /MHz						
$1.5\chi_{aa}$	-5.53732(75)	-5.539(12)	-5.552(21)	-5.525(11)	-5.562(12)	-5.562(14)
$0.25(\chi_{bb}-\chi_{cc})$	-0.07212(18)	-0.0736(15)	-0.0737(22)	-0.0747(14)	-0.0662(16)	-0.0706(17)
rms /kHz	0.87	0.80	1.13	0.75	0.85	0.87
no. lines	460	48	42	51	51	50

Table 4.2 continued

	$^{13}C_6$	$^{13}C_7$	^{15}N
Rotational Constants /MHz			
A	3342.58695(84)	3385.73955(66)	3378.01120(56)
B	1185.51849(21)	1172.08050(16)	1155.376497(96)
C	874.958222(96)	870.499331(76)	860.744972(66)
Centrifugal Distortion Constants /kHz			
Δ_J	0.0405(13)	0.0371(10)	0.03783(52)
Δ_{JK}	0.01075	0.01075	0.01075
Δ_K	1.2574	1.2574	1.2574
δ_J	0.0151(10)	0.01254(85)	0.01265(50)
δ_K	0.18152	0.18152	0.18152
^{14}N Nuclear Quadrupole Coupling Constants /MHz			
$1.5\chi_{aa}$	-5.500(14)	-5.550(11)	N/A
$0.25(\chi_{bb}-\chi_{cc})$	-0.0739(18)	-0.0691(14)	N/A
rms /kHz	0.95	0.75	0.49
no. lines	51	51	26

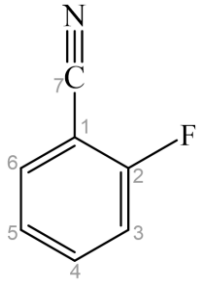
From Table 4.1 and 4.2, it is also found that while the quartic centrifugal distortion constants for the parent 2FBN and 3FBN are well determined, the Δ_K and δ_K parameters for 2FBN minor isotopologues and the Δ_{JK}, Δ_K and δ_K parameters for 3FBN minor isotopologues, were fixed at the values of the parent molecule due to the lack of high K_a transitions observed for the minor isotopic species.

4-4 Structural determination

The ground state rotational constants of the parent 2FBN and 3FBN and their minor isotopic species were used to evaluate the substitution (r_s) and effective (r_0) structures for these molecules which are shown in Table 4.3 and Table 4.4 along with the calculated *ab initio* structures. From these tables it can be seen that the substitution structures (the r_s column) for 2FBN and 3FBN are not accurately determined as the most r_s structural parameters involve large Costain errors, e.g. C2–C3 and C3–C4 bonds and C1–C2–C3 angle in 2FBN, and C1–C2 and C1–C6 distances and C1–C2–C3 angle in 3FBN.

As seen for BN in Chapter 3, the origin of the uncertainty in the substitution structures for 2FBN and 3FBN can be found by looking at their principal axis systems in Figure 4.5. In 2FBN, there is a small *a* coordinate for C2 and a small *b* coordinate for C4 and these small coordinates are accompanied by large uncertainties according to Costain's rule [6]. Further in 3FBN, the *b* coordinate for C1 is small and the *a* coordinate for C2 was calculated to be imaginary and had to be set to zero in the derivation of the internal coordinates. Therefore, the substitution (r_s) structures for 2FBN and 3FBN could not be reliably determined.

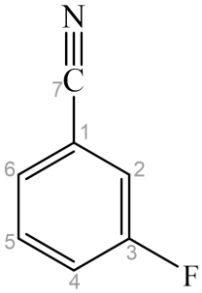
Table 4.3: The substitution (r_s), effective (r_0) and *ab initio* (r_e) structures of 2FBN (bond lengths in Ångstrom and bond angles in degrees)



Structural Parameter	r_s	r_0	r_e^{**}
C1–C2	1.357(7)	1.385(4)	1.396
C2–C3	1.422(14)	1.383(3)	1.386
C3–C4	1.378(20)	1.396(4)	1.394
C4–C5	1.416(23)	1.398(5)	1.397
C5–C6	1.399(4)	1.394(4)	1.391
C1–C6	1.396(4)	1.400(5)	1.403
C1–C7	1.449(4)	1.445(4)	1.431
C7–N	1.158(1)	1.157*	1.173
∠(C1–C2–C3)	120.2(7)	122.0(3)	121.8
∠(C2–C3–C4)	119.2(6)	118.5(4)	118.9
∠(C3–C4–C5)	120.3(2)	120.6(3)	120.4
∠(C4–C5–C6)	119.7(4)	120.0(4)	120.1
∠(C5–C6–C1)	119.0(2)	119.5(2)	120.1
∠(C6–C1–C2)	121.6(6)	119.4(3)	118.7
∠(C7–C1–C2)	119.0(6)	120.6(4)	120.4
∠(N–C7–C1)	179.1(3)	179.2(4)	178.8

* Fixed at the average C–N distance in BN and PFBN
** Calculated at MP2/6-311++G(2d,2p) level

Table 4.4: The substitution (r_s), effective (r_0) and *ab initio* (r_e) structures of 3FBN (bond lengths in Ångstrom and bond angles in degrees)



Structural Parameter	r_s	r_0	r_e^{**}
C1–C2	1.306(32)	1.401(9)	1.401
C2–C3	1.464(2)	1.386(8)	1.386
C3–C4	1.380(4)	1.383(4)	1.389
C4–C5	1.399(2)	1.395(4)	1.395
C5–C6	1.389(3)	1.401(6)	1.393
C1–C6	1.433(44)	1.392(10)	1.401
C1–C7	1.435(12)	1.446(4)	1.435
C7–N	1.158(2)	1.157*	1.173
∠(C1–C2–C3)	116.9(14)	117.1(4)	118.0
∠(C2–C3–C4)	122.3(2)	123.3(3)	122.7
∠(C3–C4–C5)	118.2(1)	118.3(8)	118.5
∠(C4–C5–C6)	120.5(1)	120.6(11)	120.7
∠(C5–C6–C1)	118.9(4)	119.0(3)	119.3
∠(C6–C1–C2)	123.2(10)	121.7(4)	120.8
∠(C7–C1–C2)	119.2(31)	118.8(8)	119.4
∠(N–C7–C1)	178.6(18)	179.7(6)	179.8

* Fixed at the average C–N distance in BN and PFBN
** Calculated at MP2/6-311++G(2d,2p) level

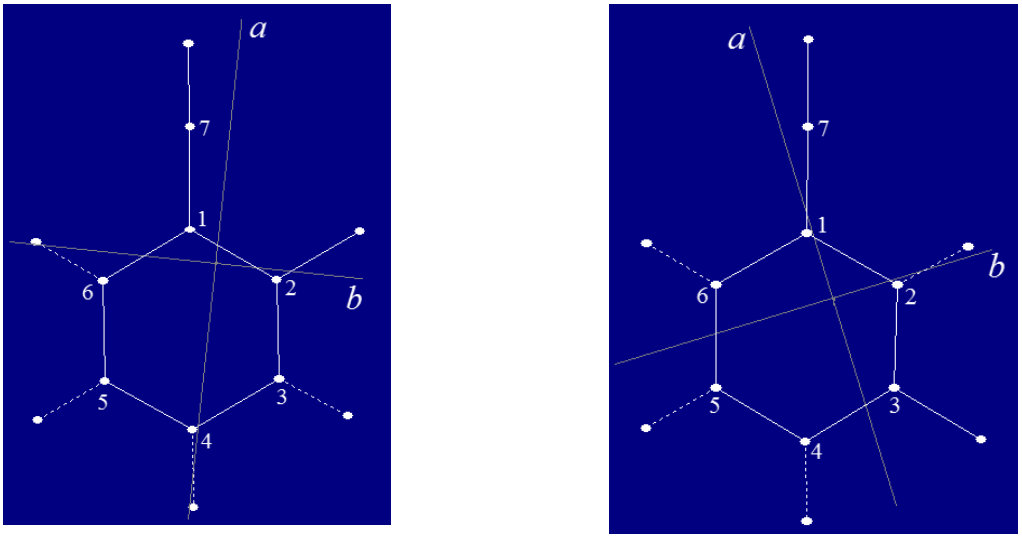


Figure 4.5: Comparison of the principal axis systems of 2FBN (left) and 3FBN (right)

From Table 4.3 and Table 4.4 it is seen that the effective (r_0) structures for 2FBN and 3FBN are more accurately determined. Usually, effective structures are reliable because they are derived from the least-squares analysis in which the selected structural parameters (bond lengths and bond angles in this case) are varied to reproduce the observed moments of inertia [7]. However, there were several problems that had to be overcome while evaluating the effective structures for 2FBN and 3FBN. First there is no isotopic substitution for the fluorine atom and the rotational spectra for deuterium substitutions could not be measured due to the very small natural abundance of ^{2}H species (0.02%, too small compared to ^{13}C species with the natural abundance of 1.11%). Further, both 2FBN and 3FBN molecules are not exactly planar in the ground state rotational constants since the inertial defect, $\Delta_0 = I_c - I_b - I_a$, has a non-zero (though small) value of 0.117 amu.Å^2 for 2FBN and 0.115 amu.Å^2 for 3FBN.

Due to the mentioned issues, the normal least-squares equations for 2FBN and 3FBN become ill-conditioned and two solutions were examined to overcome these issues. One is to add some restrictive conditions to the fit which might include holding particular structural parameters constant [7]. In the case of 2FBN and 3FBN, it was found that fixing the C7−N distance at its average distance in BN and PFBN (1.157 Å) improves the quality of the r_0 fit.

This assumption seems to be reasonable since the C7−N bond was found to remain almost the same in BN and PFBN and unaffected by the full fluorination (Chapter 3). In addition, the calculated (r_e) value of the C7−N distance (1.157 Å) is similar in BN, PFBN, 2FBN and 3FBN (and other fluorinated BN's) though the mentioned bond length differs in these derivatives by a negligible amount (<0.001Å). The second solution to improve the r_0 fit is to use the linear combinations of rotational constants such that the selected structural parameters are fitted to the observed planar moments of inertia [7-9]. In the case of 2FBN and 3FBN, the rotational constants for each isotopologue were reduced to two in which only the A and B rotational constants were used in the fit. In other words, a total of 18 experimentally determined A and B rotational constants from the parent and eight isotopologues, instead of the total of 27 determined A, B and C rotational constants in the regular r_0 fit, were used. This assumption gave satisfactory fits for the almost planar 2FBN and 3FBN.

4-5 Discussion

The effect of single fluorination at the *ortho* position on the geometry of BN can be realized by comparing the geometries of 2FBN and BN (reference compound). This comparison is shown in Figure 4.6 and is made by using the r_0 and r_e structures of 2FBN and BN in which the positive changes show the increase of bond length or bond angle and negative variations indicate the contraction of bond length or bond angle.

First, the variation of bond lengths of 2FBN is examined. Based on the δr_0 values, the most affected bonds in the ring are the adjacent bonds to the fluorination site, i.e. the C1−C2 and C2−C3 bonds, which are shortened by 0.012 Å. Similar variations for these two bonds are predicted by the MP2 theory (δr_e values).

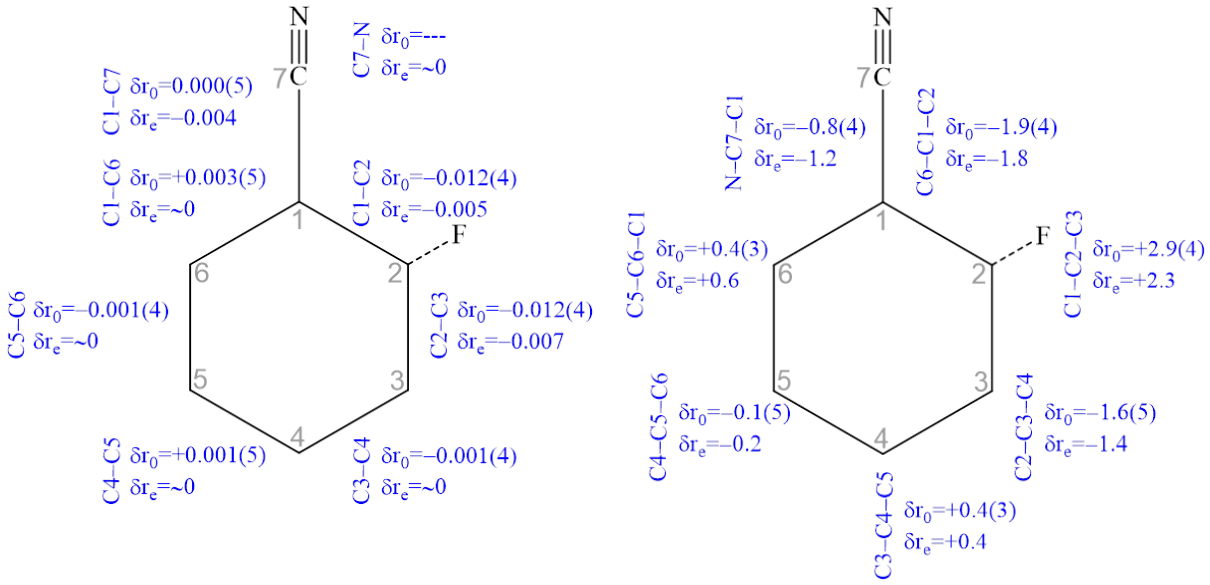


Figure 4.6: Structural changes in 2FBN as a function of single fluorination at the *ortho* position of BN based on r_0 and r_e structures and by considering BN as the reference compound. Bond length and bond angle differences are in Ångstroms and degrees, respectively.

The variations of the rest of the bonds in the ring were small compared to the experimental error margins such that the δr_0 values could not be used to monitor those small changes. Nevertheless, the δr_e values reveal that the rest of the ring bonds in 2FBN are barely distorted. For the outer C1−C7 bond, while the δr_0 value could not be used, a small contraction of 0.004 Å is predicted by the MP2 theory.

For the inner ring angles of 2FBN and based on δr_0 values, the angle at the fluorination site (C2) widens by 2.9° while the adjacent angles at C1 and C3 decrease by 1.9° and 1.6°, respectively. Subsequently the angles at C4 and C6 are associated with small opening of 0.4°. Such angular distortions are predicted from the δr_e values as well. For the remaining angle at C5, although the corresponding δr_0 value is too small compared to the error margin, the MP2 theory predicts that this angle remains undistorted.

According to the δr_0 and δr_e values, the ring geometry distortions in 2FBN can be summarized as follows: The angle at the fluorination site (C2) increases by few degrees (2−3°) whereas the adjacent angles contract by few degrees and the neighbouring C–C bonds shorten as well. The rest of the ring bonds and bond angles undergo minimal changes.

The observed geometry deformations in 2FBN can be interpreted by Bent's rule [10] and the hybridization model proposed by him as presented in Chapter 3. Based on Bent's rule, the fluorine substitution perturbs the hybridization at the fluorinated carbon such that the *p* character of the carbon σ-bonding orbital pointing towards the fluorine increases while the *p* character of the other two hybrid orbitals of carbon towards the adjacent carbon atoms decreases (the *s* character in those orbitals increases subsequently). As a result, the angle within the ring at the fluorination site (at C2) widens. The neighbouring angles at C1 and C3 contract to compensate for this change. In addition, the neighbouring C1–C2 and C2–C3 bonds shorten since there is more *s* character (less *p* character) in carbon's hybrid orbitals towards the adjacent C2 and C3 atoms. A natural bonding orbital (NBO) analysis was performed at the MP2/6-311++G(2d,2p) level of theory and the change in the carbon's hybridization via fluorination was calculated compared to the reference BN (Chapter 3). The NBO analysis results are shown in Figure 4.7, and confirm the interpretation based on Bent's rule in which the *p* character of carbon's hybrid orbital towards the fluorine increases (by 6%) and the *s* character of the other two hybrid orbitals towards the adjacent carbon atoms increases (by 3 to 4%) via fluorination.

The effect of single fluorination at the *meta* position on the geometry of BN can be understood by comparing the geometries of 3FBN and BN which is shown in Figure 4.8.

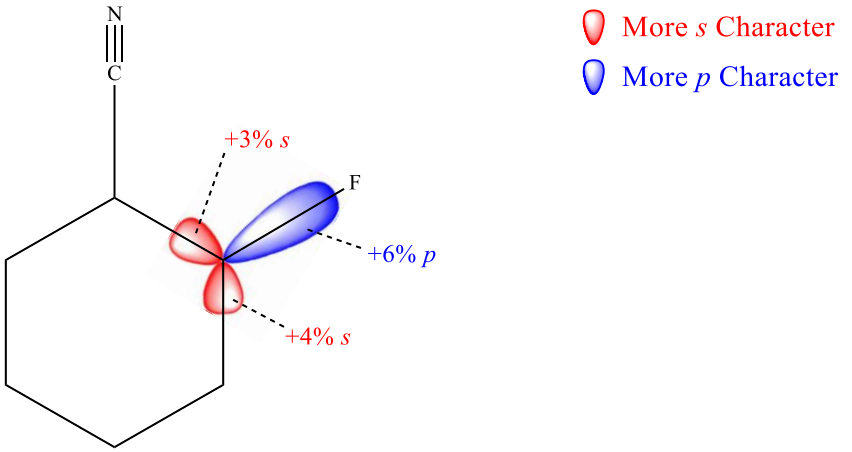


Figure 4.7: Perturbation of hybridization in 2FBN upon single fluorination at the *ortho* position according to the NBO analysis results

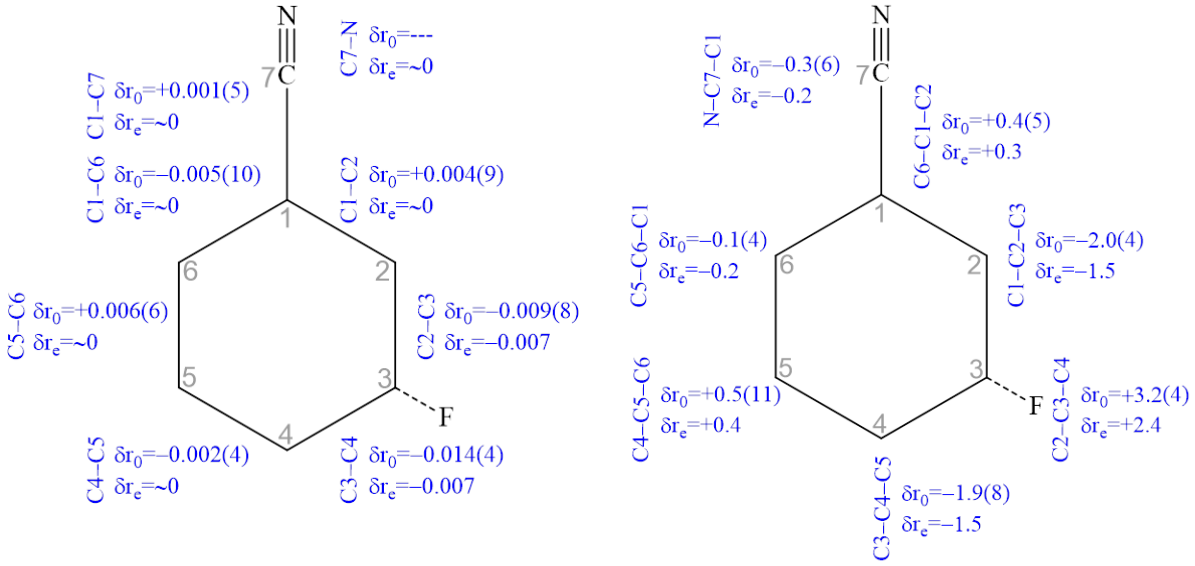


Figure 4.8: Structural changes in 3FBN as a function of single fluorination at the *meta* position of BN based on r_0 and r_e structures and by considering BN as the reference compound. Bond length and bond angle differences are in Ångstroms and degrees, respectively.

The variation of bond lengths of 3FBN is first examined. The most affected bonds in the ring are the adjacent bonds to the fluorination site, i.e. C2−C3 and C3−C4 bonds, which are shortened by 0.009 Å and 0.014 Å, respectively. Although the δr_0 value for the C2−C3 distance includes a large uncertainty of ±0.008 Å, according to the δr_e value of −0.007 Å which is the same for both C2−C3 and C3−C4 bonds, one can say that C2−C3 distance is

expected to contract to a similar extent as the C2−C3 bond. The variations of the rest of the bonds in the ring and also outside the ring (C1−C7 bond) were small compared to the experimental error margins such that the δr_0 values could not be used to monitor those small changes. Nevertheless, the δr_e values reveal that such bonds in 3FBN are barely affected by fluorination at the *meta* position.

Regarding the ring angles of 3FBN and using the δr_0 values, the angle at the fluorination site (C3) widens by 3.2° while the neighbouring angles at C2 and C4 contract by 2.0° and 1.9°, respectively. Similar changes are seen from the MP2 predictions. The variations of the remaining angles at C5, C6 and C1 cannot be monitored by the δr_0 values although the MP2 theory predicts minimal distortions for these angles.

The geometry distortions in 3FBN (according to the δr_0 and δr_e values) can be summarized as follows: The angle at the fluorination site (C3) opens by few degrees whereas the adjacent angles and also the adjacent C−C bonds contract. Fewer ring deformations are seen by going far away from the fluorinated carbon as was seen in 2FBN.

The observed geometry deformations in 3FBN can be interpreted by Bent's rule [10] in a similar manner to 2FBN. The angle at the fluorination site (at C3) opens since the *p* character of the hybridization state at the fluorinated carbon reduces. The neighbouring angles at C2 and C4 however contract to compensate. The neighbouring C2–C3 and C3–C4 bonds shorten as well as the more *s* character (less *p* character) in carbon's hybrid orbitals towards the adjacent C3 and C4 atoms results in the formation of shorter C–C bonds. As seen for 2FBN, an NBO analysis revealed the change in the carbon's hybridization at the fluorination site in 3FBN and the results are shown in Figure 4.9 which confirms the interpretation according to Bent's hybridization theory.

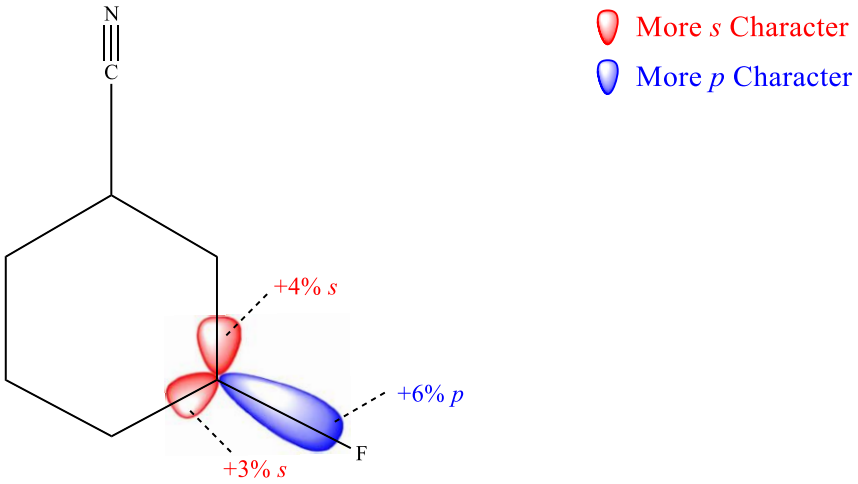


Figure 4.9: Perturbation of hybridization in 3FBN upon single fluorination at the *meta* position according to the NBO analysis results

In addition to studying the ring deformations in 2FBN and 3FBN, it is worth considering the deviation of the outer ring angle C1−C7−N in these molecules which is shown in Figure 4.10. In the cases of the previously studied BN and PFBN (Chapter 3), the mentioned angle is 180° because of the existence of a symmetry axis (C_2) in the molecule. However for 2FBN and 3FBN, the C1−C7−N angle seems to deviate from this. According to the δr_0 values for 2FBN, the C1−C7−N angle is deviated by 0.8° towards the opposite site of the fluorine atom and this small deviation is also predicted by MP2 theory with the value of δr_e=−1.2°. For 3FBN, this deviation is even smaller such that it cannot be tracked by the δr_0 values although MP2 theory predicts a very small deviation of δr_e=−0.2°.

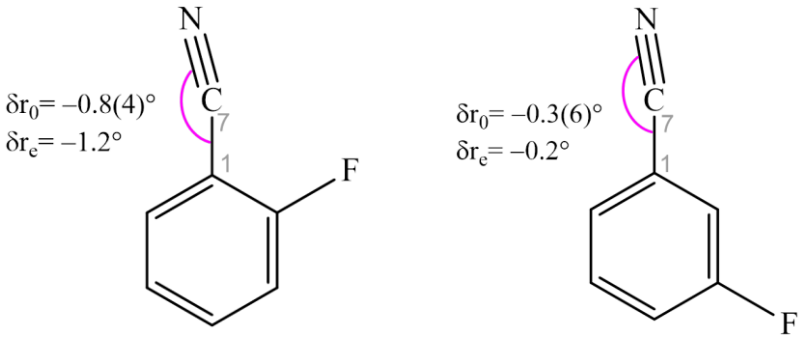


Figure 4.10: Comparison of the deviation of the C1−C7−N angle from 180° in 2FBN and 3FBN, deviations not to scale

The small deviation of the C1−C7−N angle in 2FBN can be rationalized by considering the interaction between the lone pairs (n) of electrons on the fluorine atom with the anti-bonding orbital (π*) of the adjacent cyano group. It is worth mentioning that such n→ π* interactions were found to contribute to structure and conformational preference of biologically important molecules [11-12] For instance, the interaction between the lone pairs (n) on an oxygen atom with the anti-bonding orbital (π*) of an adjacent carbonyl group resulted in stabilizing the *α*-helix protein [13].

In the case of 2FBN, a natural bonding orbital (NBO) analysis was performed at the MP2/6-311++G(2d,2p) level of theory and the second-order perturbation energies, which reflect the interactions between the donor and acceptor NBOs, were calculated. It was found that there is an interaction between the non-bonded lone pair (n) on fluorine (donor NBO) with the anti-bonding π* orbital of the C ≡ N bond (acceptor NBO) and such n→ π* interaction, which is shown in Figure 4.11, was associated with a small stabilization energy of 0.65 kcal.mol^{-1}. In addition, the analysis of the calculated natural charges showed that the F and C7 atoms have opposite signs which reveals that in addition to the orbital interaction, there is an electrostatic contribution to such a non-boding interaction.

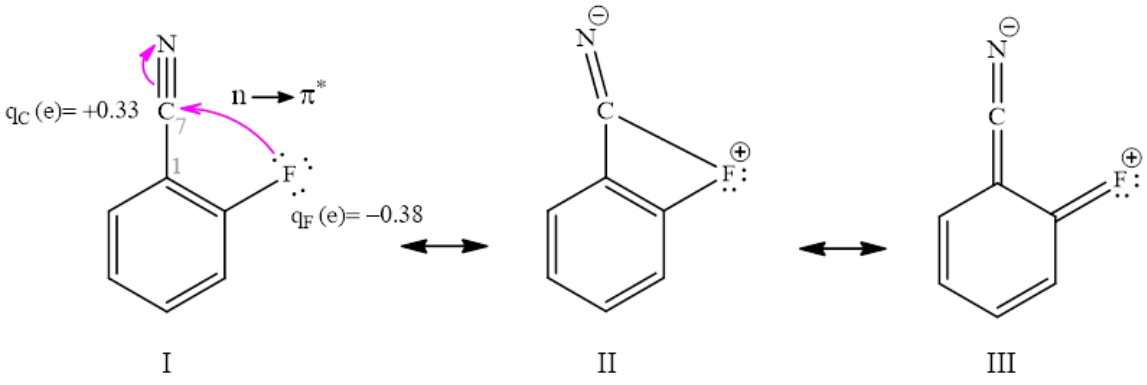


Figure 4.11: The n→ π* interaction between the donor and acceptor NBOs in 2FBN calculated at the MP2/6-311++G(2d,2p) level along with some possible resonance structures

As a result of this n→ π* interaction, a four-membered ring (resonance structure II) is formed in which the C1−C7−N angle deviates from 180° towards the opposite of the fluorine atom. The other resonance structures, e.g. resonance form III, are likely less important than the resonance form II as the aromaticity of ring is not preserved in them. It should be mentioned that although the weight of the resonance structure II is probably very small, such a small contribution can be responsible for the observed small deviation of about 1° for the C1−C7−N angle.

In summary to this chapter, the results of the MW studies for two mono-fluorinated derivatives of benzonitrile, 2FBN and 3FBN, were presented and the experimental (r_s and r_0) and theoretical (r_e) structures of these two molecules were evaluated. While the substitution (r_s) structures for both molecules could not be reliably determined, the least-squares approach resulted in more reliable r_0 structures. Comparing the geometries of 2FBN and 3FBN with that of the reference compound (BN) allowed the monitoring of structural changes caused by single fluorination at the *ortho* and *meta* positions of BN. The structural changes based on the r_0 structures, which were supported by the MP2 theory predictions, revealed that in 2FBN and 3FBN, most structural deformations are observed in the vicinity of the fluorination site and minimal distortions are seen in the opposite part of the ring to the fluorine substituent. Eventually, the observed geometry deformations caused by single fluorination were interpreted by hybridization theory and by examining the intramolecular n→ π* interactions.

In Chapter 5, the results of MW studies and structural determination for two di-fluorinated derivatives of BN: 2,3-difluorobenzonitrile and 2,4-difluorobenzonitrile will be presented. Further, the effect of double fluorination at the *ortho/meta* and *ortho/para* positions on the geometry of BN will be discussed in relation to the results for single (Chapter 4) and full (Chapter 3) fluorination.

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Chapter 5: Microwave study and molecular structure of 2,3-difluorobenzonitrile and 2,4-difluorobenzonitrile

In this chapter, the results of MW studies and structural determination for two di-fluorinated derivatives of benzonitrile including 2,3-difluorobenzonitrile (23DFBN) and 2,4-difluorobenzonitrile (24DFBN) are presented. In addition, the effect of double fluorination at the *ortho/meta* and *ortho/para* positions on the geometry of BN are discussed.

5-1 Introduction

The molecular structures of 23DFBN and 24DFBN and their principal axis systems are shown in Figure 5.1 and Figure 5.2. These planar molecules have the point group of C_s. The 23DFBN molecule has an estimated dipole moment of 5.64 D [at MP2/6-311++G(2d,2p) level] with components of μ_A = 3.94 D and μ_B = 4.03 D and therefore strong *a*- and *b*-type rotational transitions are expected for this species. The total dipole moment of 24DFBN is calculated to be 4.27 D at the same level of theory with components of μ_A = 4.13 D and μ_B = 1.08 D and hence strong *a*-type and weaker *b*-type rotational transitions are anticipated for this molecule.

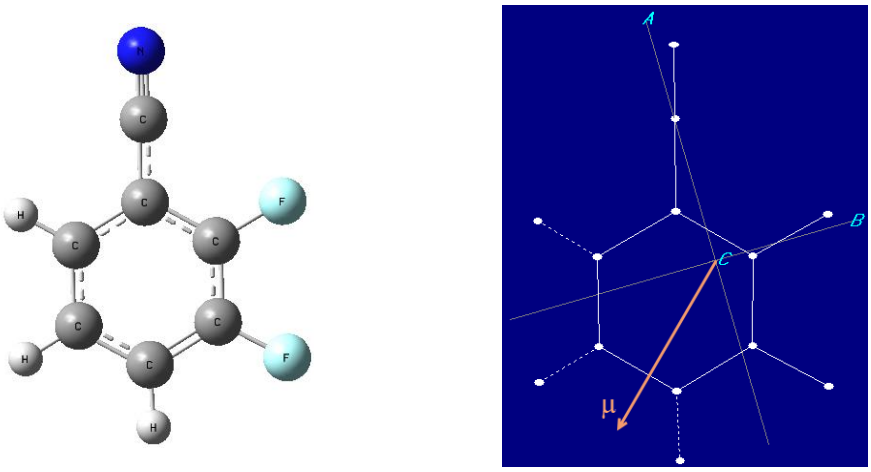


Figure 5.1: Molecular structure and principal axis system of 23DFBN

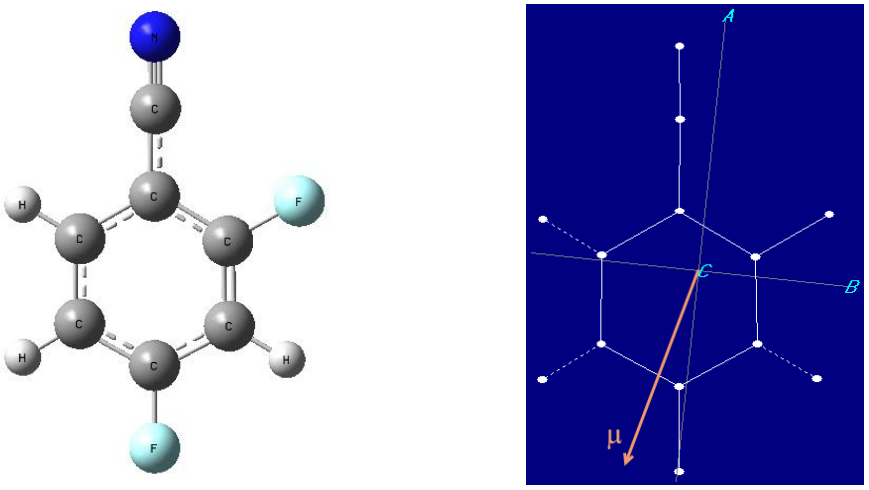


Figure 5.2: Molecular structure and principal axis system of 24DFBN

For 23DFBN and 24DFBN, there are seven different carbon atoms in terms of chemical environment and therefore there are seven unique ^{13}C and one ^{15}N isotopologues for these molecules which all show weak rotational transitions in the MW spectrum due to the small natural abundance of ^{13}C and one ^{15}N isotopically substituted species.

The MW spectrum of 23DFBN was first studied by Maiti et al. in 1990 using a Stark modulated MW technique. From that work, the rotational constants of the parent 23DFBN were evaluated and an approximate r_0 structure was proposed based on the reproduction of the observed principal moments of inertia of the parent species [1]. Later on in 2002, the higher resolution FTMW technique was used to determine the rotational constants and ^{14}N nuclear quadrupole coupling constants of the parent 23DFBN [2]. Eventually in 2006, the frequency range of investigation was extended to the millimetre-wave region and by assigning the rotational transitions due to the higher J and K_a values, accurate values of centrifugal distortion constants for the parent species were evaluated [3].

To date, although the MW spectrum of the parent 23DFBN is known, the MW spectra of the minor isotopic species, which are required to evaluate the accurate experimental structure, have not been investigated. In this work, the rotational spectrum of the parent 23DFBN was

reinvestigated in which the range of high resolution spectral measurements was extended from 4 to 26 GHz and many new transitions were collected which allowed the precise determination of spectroscopic constants of the parent species including the rotational constants, centrifugal distortion parameters and ^{14}N nuclear quadrupole coupling constants. In addition to the parent 23DFBN, the high resolution MW spectra of the minor ^{13}C and ^{15}N isotopic species were investigated in the same frequency region for the first time and the newly derived experimental (r_s and r_0) structures are reported.

Regarding 24DFBN, there have been no MW studies on this molecule to date and in this work, the rotational spectra of the parent 24DFBN and its ^{13}C and ^{15}N isotopologues are investigated for the first time and the newly evaluated substitution (r_s) and effective (r_0) structures are reported for this species.

5-2 Experimental details

The pure liquid 23DFBN (98%) and pure solid 24DFBN (97%) were purchased from Sigma-Aldrich. 2 bars of argon was used as the carrier gas and was introduced into a bubbler containing the sample while the bubbler was placed in a heating bath fixed at the temperature of 60 °C to increase the sample's vapor pressure and also to melt the solid 24DFBN sample. For 23DFBN, the pure rotational spectra of the parent species was reinvestigated by the FTMW instrument in the 4 to 26 GHz region in which some rotational transitions were re-measured and many new transitions were collected. In addition to the parent species, the high resolution MW spectra of the ^{13}C and ^{15}N isotopologues were measured with the FTMW instrument in the 4 to 26 GHz region. For 24DFBN, since there were no previous MW studies, some broadband MW spectra were recorded using the cp-FTMW instrument to initially assign the rotational transitions due to the parent species and then the high resolution

MW spectra of the parent 24DFBN and its minor isotopologues were collected with the FTMW instrument in the 4 to 26 GHz region.

5-3 Spectral assignment and fitting

The MW spectrum of 23DFBN included strong *a*- and *b*-type rotational transitions which arose from the large values of dipole moment components (μ_A = 3.94 D and μ_B = 4.03 D). A sample high resolution MW spectrum for the parent 23DFBN is shown in Figure 5.3. A total of 93 *a*-type and 71 *b*-type transitions (and their hyperfine components) were measured for the parent 23DFBN spanning J=2 to J=13 and no less than 13 *a*-type and 9 *b*-type transitions (and their hyperfine components) were collected for the minor isotopic species. It has to be mentioned that for the 23DFBN isotopologues, both *a*- and *b*-type transitions were observable due to the large values of dipole moment components μ_A and μ_B. The fitted spectroscopic constants for the parent 23DFBN and its minor isotopic species, obtained from the Watson's A-reduced Hamiltonian (I^r representation), are filled in Table 5.1 and the measured rotational transitions are listed in Appendix V.

The 24DFBN spectrum showed strong *a*-type and weaker *b*-type transitions as predicted from the calculated values of dipole moment components (μ_A = 4.13 D and μ_B = 1.08 D). A survey broadband MW spectrum from the cp-FTMW instrument is illustrated in Figure 5.4 in which some of the rotational transitions of the parent 24DFBN (mostly *a*-type transitions) are shown. A sample spectrum from the FTMW instrument is also demonstrated in Figure 5.5. A number of 106 *a*-type and 24 *b*-type transitions (and their hyperfine components) were measured for the parent 24DFBN spanning J=4 to J=15 and a minimum of 17 *a*-type transitions (and their hyperfine components) were collected for the minor isotopologues. It is worth mentioning that for the 24DFBN minor isotopic species, the *b*-type transitions were not

observable as both the μ_B dipole component and natural abundance of these species are small. By fitting the measured rotational transitions to the same Hamiltonian model as for 23DFBN, the spectroscopic constants for the parent 24DFBN and its minor isotopologues were evaluated for the first time which are illustrated in Table 5.2. The observed rotational transitions are provided in Appendix VI.

As seen for BN and PFBN (Chapter 3), and 2FBN and 3FBN (Chapter 4), the trends in the spectroscopic constants for the parent molecule and minor isotopologues of 23DFBN and 24DFBN, as shown in Table 5.1 and 5.2, are similar. From these tables it can also be found that while the quartic centrifugal distortion constants for the parent 23DFBN and 24DFBN are well determined, the Δ_K parameter for the 23DFBN minor isotopologues and the Δ_K and δ_J parameters for the 24DFBN minor isotopologues, were fixed at the values of the parent molecule due to the lack of high K_a transitions observed for the minor isotopic species.

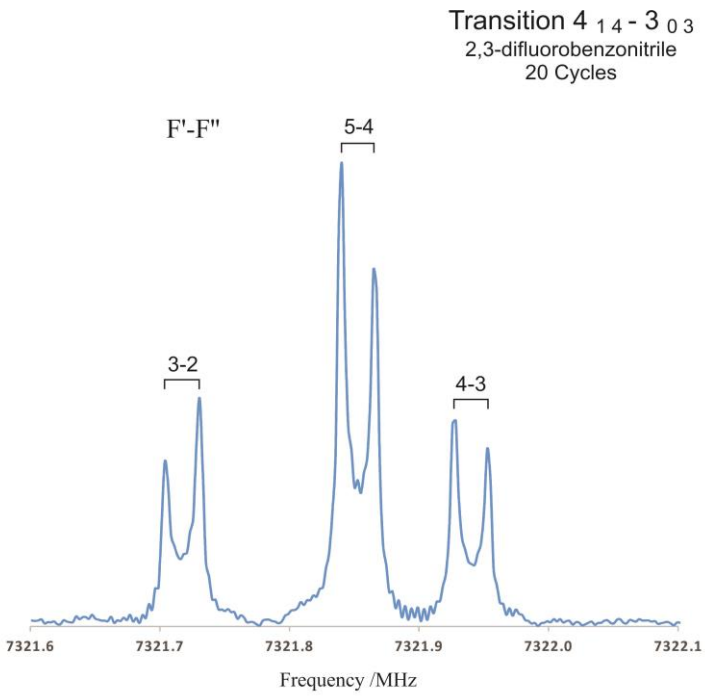


Figure 5.3: Sample FTMW spectrum of the 4 $_{1\,4}$ - 3 $_{0\,3}$ rotational transition of 23DFBN showing the hyperfine splitting arising from the ^{14}N quadrupolar nucleus

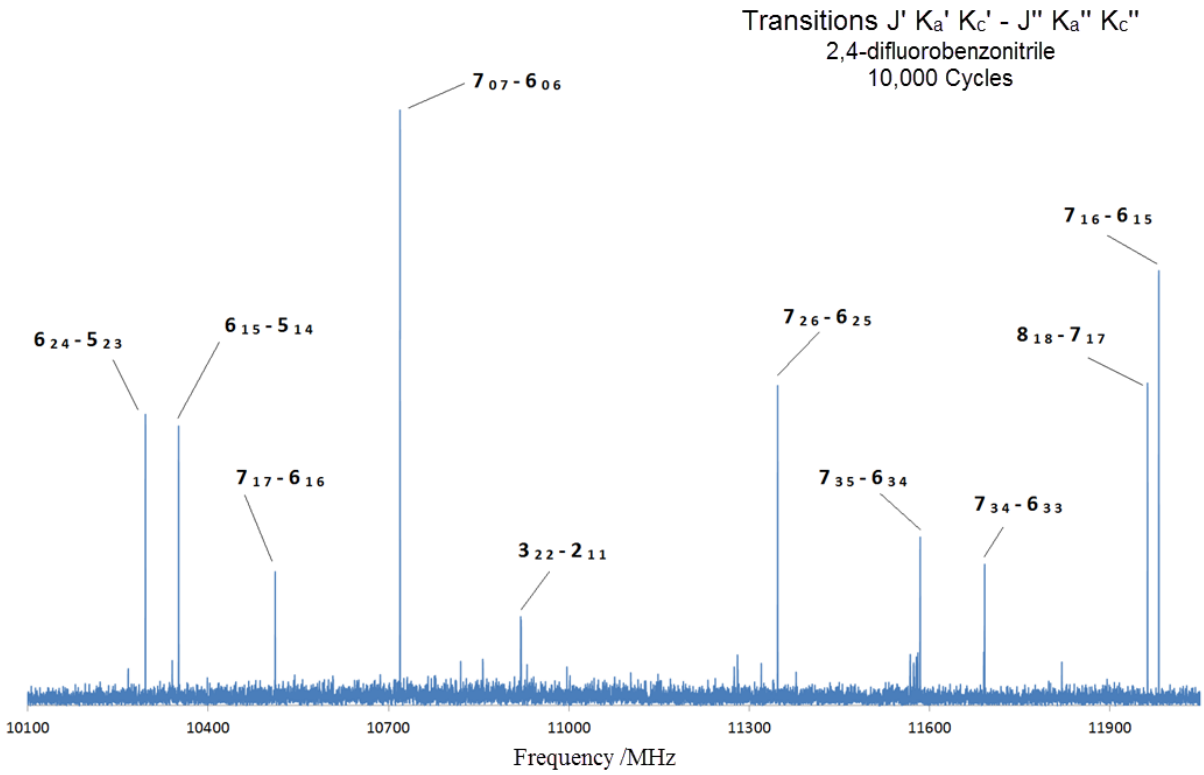


Figure 5.4: Sample cp-FTMW spectrum of 24DFBN showing some of the rotational transitions of the parent species

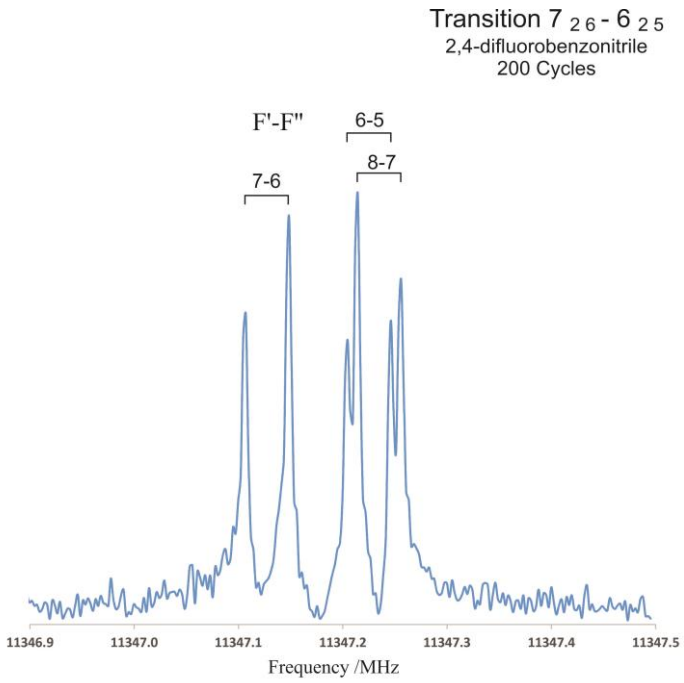


Figure 5.5: Sample FTMW spectrum of the 7 $_{26}$ - 6 $_{25}$ rotational transition of 24DFBN showing the hyperfine splitting arising from the ^{14}N quadrupolar nucleus

Table 5.1: Spectroscopic constants of 23DFBN and its minor isotopic species

	Normal	$^{13}C_1$	$^{13}C_2$	$^{13}C_3$	$^{13}C_4$	$^{13}C_5$
Rotational Constants /MHz						
A	2260.152021(47)	2258.73587(84)	2256.79214(88)	2259.81277(73)	2247.48305(89)	2216.33857(72)
B	1182.866459(15)	1180.64140(20)	1182.89578(21)	1177.28393(18)	1174.06050(22)	1181.13493(18)
C	776.3845304(91)	775.259812(78)	776.000957(84)	773.936658(68)	771.095766(85)	770.409716(69)
Centrifugal Distortion Constants /kHz						
Δ_J	0.034910(91)	0.0359(16)	0.0357(15)	0.0346(14)	0.0347(18)	0.0331(14)
Δ_{JK}	0.17894(45)	0.164(15)	0.173(19)	0.157(13)	0.174(16)	0.183(13)
Δ_K	-0.0479(27)	-0.0479	-0.0479	-0.0479	-0.0479	-0.0479
δ_J	0.012851(41)	0.01320(88)	0.01304(88)	0.01231(79)	0.01268(98)	0.01179(79)
δ_K	0.16072(59)	0.168(13)	0.174(18)	0.157(12)	0.168(14)	0.155(11)
^{14}N Nuclear Quadrupole Coupling Constants /MHz						
$1.5\chi_{aa}$	-5.80400(76)	-5.7902(88)	-5.8036(94)	-5.7986(79)	-5.8469(98)	-5.8597(79)
$0.25(\chi_{bb}-\chi_{cc})$	-0.03156(20)	-0.0339(16)	-0.0311(14)	-0.0335(14)	-0.0235(17)	-0.0235(13)
rms /kHz	0.92	0.91	0.89	0.82	1.02	0.81
no. lines	512	70	66	71	78	75

Table 5.1 continued

	$^{13}C_6$	$^{13}C_7$	^{15}N
Rotational Constants /MHz			
A	2230.08374(72)	2260.14605(70)	2259.19886(36)
B	1182.01545(18)	1168.65567(17)	1151.97324(10)
C	772.441013(68)	770.236572(67)	762.842501(40)
Centrifugal Distortion Constants /kHz			
Δ_J	0.0363(14)	0.0352(14)	0.03396(88)
Δ_{JK}	0.160(13)	0.166(12)	0.1802(58)
Δ_K	-0.0479	-0.0479	-0.0479
δ_J	0.01390(80)	0.01312(77)	0.01226(47)
δ_K	0.163(11)	0.160(11)	0.1628(69)
^{14}N Nuclear Quadrupole Coupling Constants /MHz			
$1.5\chi_{aa}$	-5.7847(79)	-5.8140(79)	N/A
$0.25(\chi_{bb}-\chi_{cc})$	-0.0355(13)	-0.0335(12)	N/A
rms /kHz	0.82	0.81	0.32
no. lines	78	76	35

Table 5.2: Spectroscopic constants of 24DFBN and its minor isotopic species

	Normal	$^{13}C_1$	$^{13}C_2$	$^{13}C_3$	$^{13}C_4$	$^{13}C_5$
Rotational Constants /MHz						
A	2932.25879(29)	2929.6345(30)	2919.9801(22)	2914.4249(32)	2932.1089(36)	2899.6702(28)
B	933.040695(22)	931.640706(76)	932.890874(55)	931.144425(81)	927.302693(92)	930.137616(71)
C	707.757622(15)	706.800334(65)	706.953983(48)	705.626227(69)	704.442451(81)	704.180166(62)
Centrifugal Distortion Constants /kHz						
Δ_J	0.013351(51)	0.01332(59)	0.01340(46)	0.01292(63)	0.01350(72)	0.01321(56)
Δ_{JK}	0.15649(40)	0.161(15)	0.149(11)	0.135(16)	0.130(18)	0.138(14)
Δ_K	0.728(51)	0.728	0.728	0.728	0.728	0.728
δ_J	0.003326(31)	0.003326	0.003326	0.003326	0.003326	0.003326
δ_K	0.1046(19)	0.110(30)	0.102(23)	0.095(33)	0.099(37)	0.079(29)
^{14}N Nuclear Quadrupole Coupling Constants /MHz						
$1.5\chi_{aa}$	-6.2974(21)	-6.286(13)	-6.289(10)	-6.300(14)	-6.306(16)	-6.284(13)
$0.25(\chi_{bb}-\chi_{cc})$	0.09446(61)	0.0983(34)	0.0982(26)	0.1014(38)	0.0945(41)	0.0981(32)
rms /kHz	0.92	0.85	0.64	0.91	1.03	0.82
no. lines	383	54	53	54	54	54

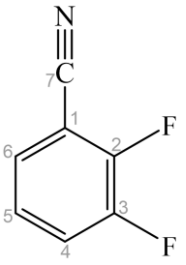
Table 5.2 continued

	$^{13}C_6$	$^{13}C_7$	^{15}N
Rotational Constants /MHz			
A	2892.9044(30)	2927.4448(31)	2925.0158(16)
B	933.046503(83)	923.757746(81)	912.733657(42)
C	705.445021(71)	702.126849(70)	695.599885(26)
Centrifugal Distortion Constants /kHz			
Δ_J	0.01336(66)	0.01317(62)	0.01288(30)
Δ_{JK}	0.140(18)	0.145(17)	0.1534(86)
Δ_K	0.728	0.728	0.728
δ_J	0.003326	0.003326	0.003326
δ_K	0.099(35)	0.087(33)	0.096(13)
^{14}N Nuclear Quadrupole Coupling Constants /MHz			
$1.5\chi_{aa}$	-6.300(21)	-6.296(20)	N/A
$0.25(\chi_{bb}-\chi_{cc})$	0.1008(35)	0.0962(36)	N/A
rms /kHz	0.85	0.86	0.31
no. lines	49	52	23

5-4 Structural determination

The ground state rotational constants of the parent 23DFBN and 24DFBN and their minor isotopic species were used to evaluate the experimental (r_s and r_0) structures for these molecules which are shown in Table 5.3 and Table 5.4 along with the calculated *ab initio* structures.

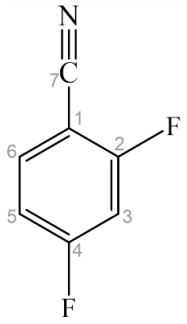
Table 5.3: The substitution (r_s), effective (r_0) and *ab initio* (r_e) structures of 23DFBN (bond lengths in Ångstrom and bond angles in degrees)



Structural Parameter	r_s	r_0	r_e**
C1–C2	1.310(4)	1.386(6)	1.395
C2–C3	1.479(3)	1.393(6)	1.391
C3–C4	1.366(8)	1.375(6)	1.386
C4–C5	1.400(2)	1.397(4)	1.397
C5–C6	1.387(3)	1.400(7)	1.391
C1–C6	1.409(4)	1.404(8)	1.403
C1–C7	1.441(18)	1.437(4)	1.431
C7–N	1.157(17)	1.157*	1.173
∠(C1–C2–C3)	117.9(4)	119.7(4)	120.0
∠(C2–C3–C4)	120.8(4)	121.5(5)	120.9
∠(C3–C4–C5)	118.9(1)	119.0(4)	119.3
∠(C4–C5–C6)	120.4(1)	120.5(5)	120.5
∠(C5–C6–C1)	119.7(2)	119.4(3)	119.9
∠(C6–C1–C2)	122.5(2)	119.9(3)	119.5
∠(C7–C1–C2)	117.3(25)	120.1(6)	119.6
∠(N–C7–C1)	179.0(57)	179.3(6)	178.8

* Fixed at the average C–N distance in BN and PFBN
** Calculated at MP2/6-311++G(2d,2p)

Table 5.4: The substitution (r_s), effective (r_0) and *ab initio* (r_e) structures of 24DFBN (bond lengths in Ångstrom and bond angles in degrees)



Structural Parameter	r_s	r_0	r_e**
C1–C2	1.387(4)	1.389(5)	1.396
C2–C3	1.357(5)	1.374(4)	1.385
C3–C4	1.371(13)	1.390(3)	1.387
C4–C5	1.409(15)	1.389(3)	1.389
C5–C6	1.306(1)	1.394(12)	1.390
C1–C6	1.455(3)	1.402(7)	1.402
C1–C7	1.440(2)	1.438(3)	1.430
C7–N	1.158(1)	1.157*	1.173
∠(C1–C2–C3)	123.5(3)	122.7(2)	122.1
∠(C2–C3–C4)	117.4(4)	117.0(3)	117.5
∠(C3–C4–C5)	122.8(2)	123.1(3)	122.7
∠(C4–C5–C6)	118.3(3)	118.2(6)	118.5
∠(C5–C6–C1)	122.4(1)	120.2(4)	120.7
∠(C6–C1–C2)	115.6(2)	118.8(4)	118.5
∠(C7–C1–C2)	121.7(3)	121.1(4)	120.5
∠(N–C7–C1)	179.2(3)	179.3(5)	178.9

* Fixed at the average C–N distance in BN and PFBN
** Calculated at MP2/6-311++G(2d,2p)

It can be found from Table 5.3 and Table 5.4 that the substitution structures for 23DFBN and 24DFBN (the r_s column) are not accurately determined as some structural parameters contain large uncertainties, e.g. C1–C7 and C7–N distances and N–C7–C1 angle in 23DFBN, and C3−C4 and C4−C5 bonds in 24DFBN.

As seen for BN in Chapter 3 and for 2FBN and 3FBN in Chapter 4, the reason for the large uncertainties and inaccuracy in the r_s structural parameters for 23DFBN and 24DFBN can be found by looking at their principal axis systems in Figure 5.6. The *b* coordinate for C7 in 23DFBN and that for C4 in 24DFBN is small, and the *a* coordinate for C2 in 23DFBN and that for C6 in 24DFBN was calculated to be imaginary and had to be set to zero in the derivation of the internal coordinates. For this reason, the r_s structural parameters for both molecules could not be accurately determined.

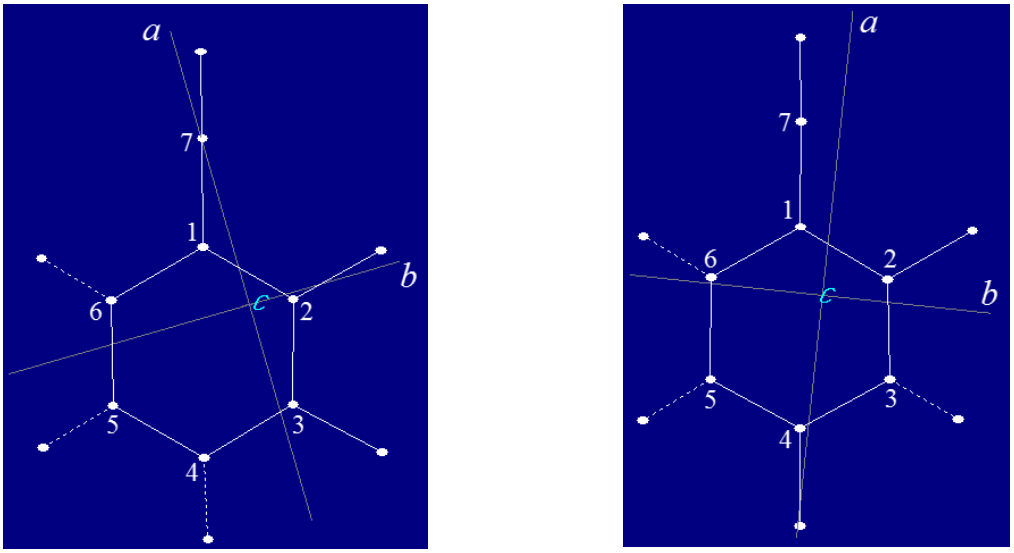


Figure 5.6: Comparison of the principal axis systems of 23DFBN (left) and 24DFBN (right)

The effective structures for 23DFBN and 24DFBN (the r_0 column in Table 5.3 and Table 5.4) are more accurately determined compared to the substitution structures because of using a least-squares approach in which the selected structural parameters (bond lengths and bond

angles in this case) are varied to reproduce the observed moments of inertia [4]. As seen for 2FBN and 3FBN in Chapter 4, there were some problems which affected the quality of the normal r_0 fit for 23DFBN and 24DFBN. The absence of an additional stable isotope for the fluorine atom and the lack of rotational spectra for deuterium substitutions are among them. In addition, both 23DFBN and 24DFBN molecules are not exactly planar in the ground state rotational constants because of having a non-zero value of the inertial defect (Δ_0) of 0.086 amu.Å^2 for 23DFBN and 0.058 amu.Å^2 for 24DFBN. Although such inertial defect values are small, they are sufficient to reduce the quality of the least-squares fit.

The mentioned issues resulted in an ill-conditioning in the normal least-squares equations for the 23DFBN and 24DFBN molecules. To overcome these issues, two solutions were examined as were described previously for 2FBN and 3FBN; First was to fix the C−N bond at the constant value of 1.157 Å (the average C−N distance in BN and PFBN) and the second solution was to reduce the number of rotational constants used in the fit to two for each isotopologue (only A and B rotational constants) [4-6]. These assumptions improved the quality of the r_0 fit for 23DFBN and 24DFBN molecules.

5-5 Discussion

To realize the effect of double fluorination at the *ortho* and *meta* positions on the geometry of benzonitrile, the r_0 and r_e structures of 23DFBN were compared to those of the reference compound (BN). In this comparison, which is shown in Figure 5.7, the positive changes show the increasing of a bond length or bond angle and negative variations indicate the contraction of a bond length or bond angle.

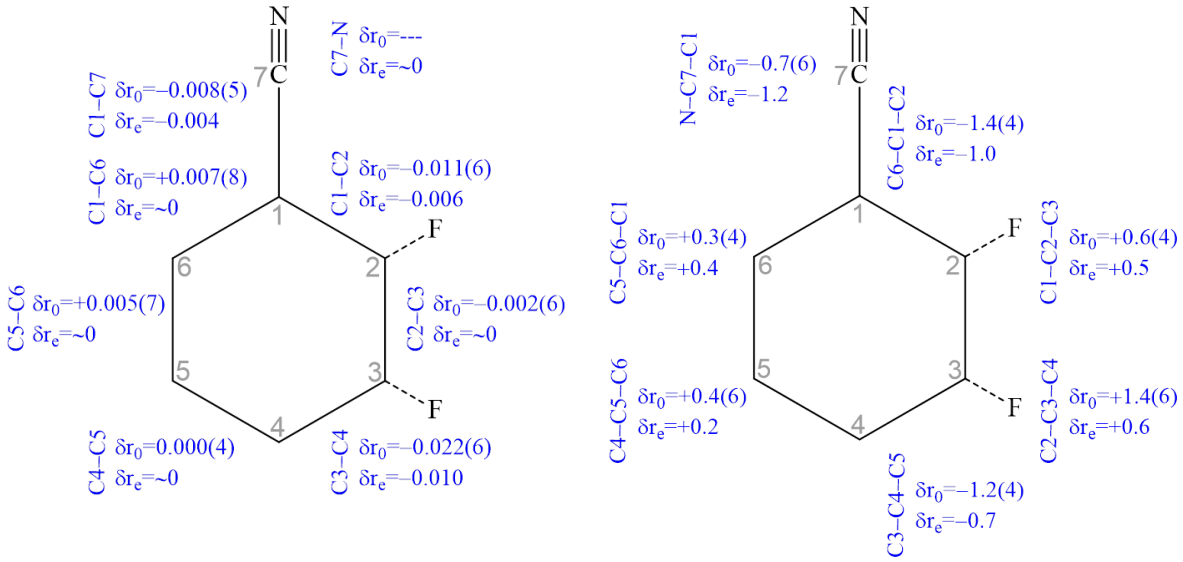


Figure 5.7: Structural changes in 23DFBN as a function of double fluorination at the *ortho/meta* positions of BN based on r_0 and r_e structures and by considering BN as the reference compound. Bond length and bond angle differences are in Ångstroms and degrees, respectively.

First the variation of bond lengths of 23DFBN is examined. Based on the δr_0 values, most distorted bonds in the ring are adjacent bonds to the fluorination sites, i.e. C1−C2 and C3−C4 distances, which are shortened by 0.011 Å and 0.022 Å, respectively. The contraction of these two bonds is predicted by the MP2 theory as well (δr_e values). The variations of the other bonds in the ring are either small or moderate such that the relatively large uncertainties in the δr_0 values do not allow one to track such changes. Nevertheless, according to the δr_e values, all the ring bonds, except for C1−C2 and C3−C4 distances which are shortened, remain unaffected. For the C1−C7 distance, a slight shortening of 0.008 Å is observed which is confirmed by the corresponding δr_e value.

For the ring angles of 23DFBN and according to the δr_0 values, the angles at the fluorination sites, i.e. at C2 and C3, widen by 0.6° and 1.4°, respectively while the adjacent angles at C1 and C4 decrease by 1.4° and 1.2°, accordingly. The rest of the angles at C5 and C6 remain almost unaffected. Similar ring angle variations in 23DFBN are predicted by MP2 theory as well.

The ring geometry distortions in 23DFBN (based on both δr_0 and δr_e values) can be summarized as follows: The angles at the fluorination sites increase by few degrees whereas the adjacent angles contract by few degrees and the neighbouring C–C bonds (except for the distance between the fluorinated carbons) shorten as well. The rest of the ring angles and ring bonds undergo minimal changes.

These distortions in 23DFBN can be explained based on Bent's hybridization theory [7] as used for PFBN in Chapter 3 and for 2FBN and 3FBN in Chapter 4. In 23DFBN, the fluorine atoms perturb the hybridizations at the fluorinated carbons which cause an increase in the *p* character of the carbon hybrid orbital pointing towards the fluorine atom and a decrease in the *p* character (increase in the *s* character) of the other two hybrid orbitals of carbon towards the adjacent carbon atoms. As a result, the angles within the ring at the fluorination sites (at C2 and C3) widen while the neighbouring angles at C1 and C4 contract to compensate for these changes. The neighbouring C1–C2 and C3–C3 bonds shorten as well due to the more *s* character in the hybrid orbitals of the fluorinated carbons that are directed towards adjacent C1 and C4 atoms. Nevertheless, it seems that the hybridization theory cannot justify the fact that the distance between the fluorinated carbons (C2−C3) is not distorted.

An NBO analysis was performed at the MP2/6-311++G(2d,2p) level of theory to evaluate the hybridization at the fluorination sites in 23DFBN and the results are shown in Figure 5.8. It is seen that the increase in the *p* character of the carbons' valences towards the fluorine atoms (by 6%) and the increase in the *s* character of the remaining two hybrid orbitals towards the adjacent carbons (by 2 to 4%), confirms the above interpretation based on Bent's hybridization theory.

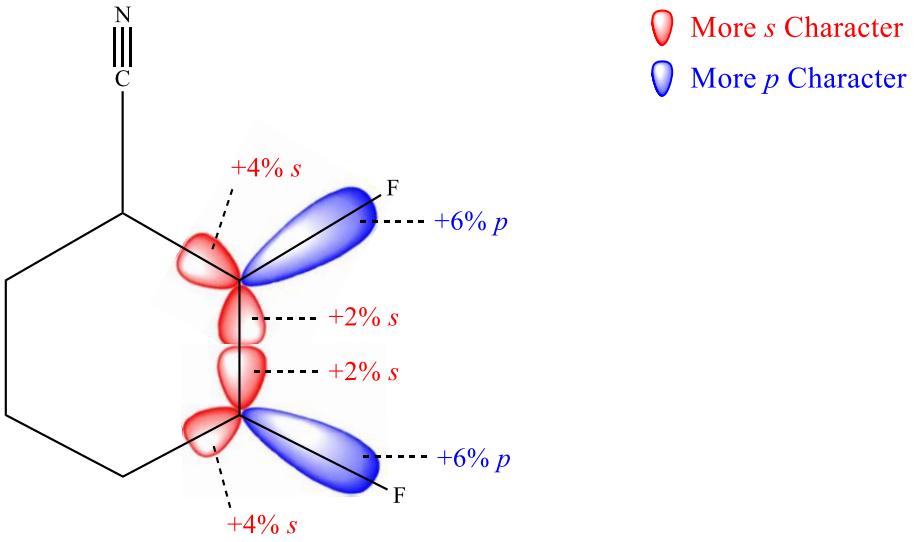


Figure 5.8: Perturbation of hybridization in 23DFBN upon fluorination at the *ortho* and *meta* positions according to the NBO analysis results

The distortion of the 23DFBN ring can also be interpreted based on the additivity of effects of the two fluorine atoms. In this molecule, the two fluorine atoms are substituted in proximity and both tend to increase the angle at their substitution sites and to decrease their neighboring angles. According to the δr_0 values, the extent of the reduction of neighboring angles at C1 and C4 in 23DFBN is close to that observed for the mono-fluorinated BNs (Chapter 4) however, the extent of the widening of angles at the fluorination sites in 23DFBN (0.6° and 1.4°) is less than that in mono-fluorinated BNs (2.9° in 2FBN and 3.2° in 3FBN). The reason for this could be that while the angle at one fluorination site (e.g. at C2) tend to open, there is an inductive effect imposed by another fluorine atom at C3 which tends to decrease the angle at the neighboring C2. The same situation happens while opening of the angle at C3 and the resultant is the less widening of the angles at the fluorination sites compared to that seen in the mono-fluorinated derivatives. In other words, the angular distortions in 23DFBN arise from the superimposition of the independent effects from each fluorine atom as observed in the related fluorinated benzenes including 1,2-difluorobenzene [8]. Such superimposition effects are not convincing for bond lengths, i.e. while the

neighboring C1–C2 and C3–C4 distances are shortened (as observed for the neighboring bonds in 2FBN and 3FBN), the C2–C3 bond seems to remain unaffected as similarly observed in 1,2-difluorobenzene [8].

The effect of double fluorination at the *ortho* and *para* positions on the geometry of benzonitrile can be realized by comparing the r_0 and r_e structures of 24DFBN with those of the reference compound (BN) which is shown in Figure 5.9.

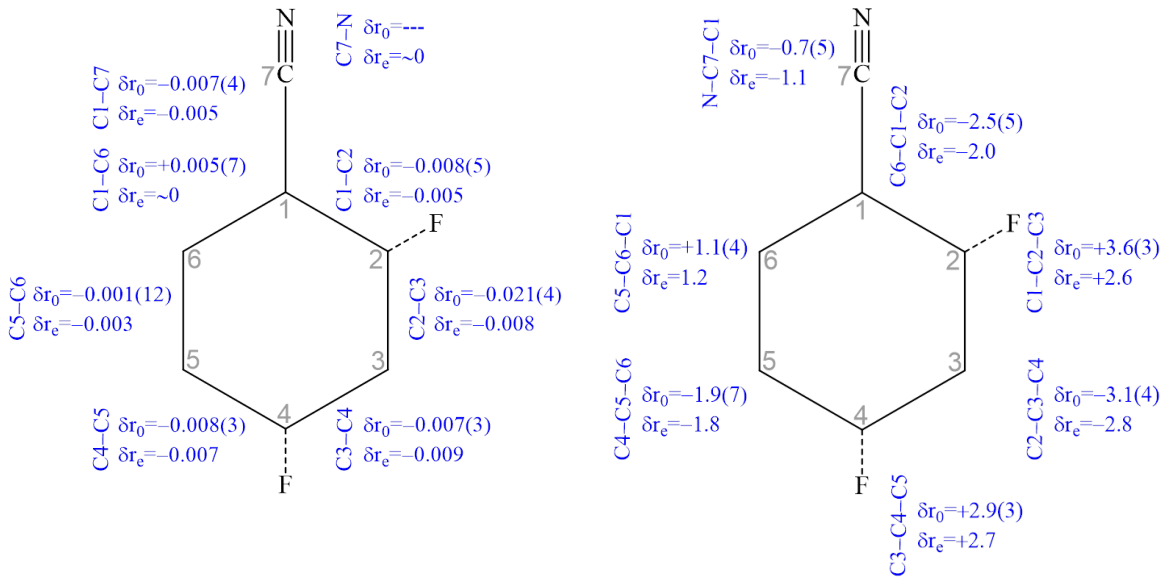


Figure 5.9: Structural changes in 24DFBN as a function of double fluorination at the *ortho/para* positions of BN based on r_0 and r_e structures and by considering BN as the reference compound. Bond length and bond angle differences are in Ångstroms and degrees, respectively.

The variation of bond lengths of 24DFBN is first examined. According to the δr_0 values, the most distorted bonds in the ring are the adjacent bonds to the fluorination sites, i.e. the C1−C2, C2−C3, C3−C4 and C4−C5 distances which are shortened by 0.008 Å, 0.021 Å, 0.007 Å and 0.008 Å, respectively. Similar variations for these bonds are predicted by MP2 theory. The variations of the remaining two bonds, C1−C6 and C5−C6, cannot be monitored by the δr_0 values, however, the MP2 theory predicts that the mentioned bonds remain almost

unaffected. Regarding the C1−C7 distance, a slight contraction of 0.007 Å is observed which is confirmed by the corresponding δr_e value.

For the inner ring angles of 24DFBN and based on δr_0 values, the angles at the fluorination sites, i.e. at C2 and C4, widen by 3.6° and 2.9°, respectively while the adjacent angles at C1, C3 and C5 contract by 2.5°, 3.1° and 1.9°, accordingly. For the remaining angle at C6, the smaller extent of opening by 1.1° was observed. The observed angular distortions in 24DFBN are supported by the MP2 theory predictions.

The ring distortions in 24DFBN (based on both δr_0 and δr_e values) can be summarized as follows: The angles at the fluorination sites increase by few degrees whereas the adjacent angles contract by few degrees and the neighbouring C–C bonds shorten as well. It also appears as though the effects are not localized around the sites of fluorination which was not observed for the other species.

The observed ring deformations in 24DFBN can be interpreted by Bent's hybridization theory [7] in a similar manner to 23DFBN and the other fluorinated benzonitriles. A schematic of the perturbation of hybridization in 24DFBN, according to an NBO analysis performed at the same level of theory as for 23DFBN, is shown in Figure 5.10. The angles at the fluorination sites (at C2 and C4) open due to decrease in the *p* character of the hybridization state at the fluorinated carbons. The neighbouring angles at C1, C3 and C5 however contract to compensate for these changes. The neighbouring C1−C2, C2−C3, C3−C4 and C4−C5 bonds shorten as well because of the more *s* character (less *p* character) in the hybrid orbitals of the fluorinated carbons which are towards the adjacent C1, C3 and C5 atoms.

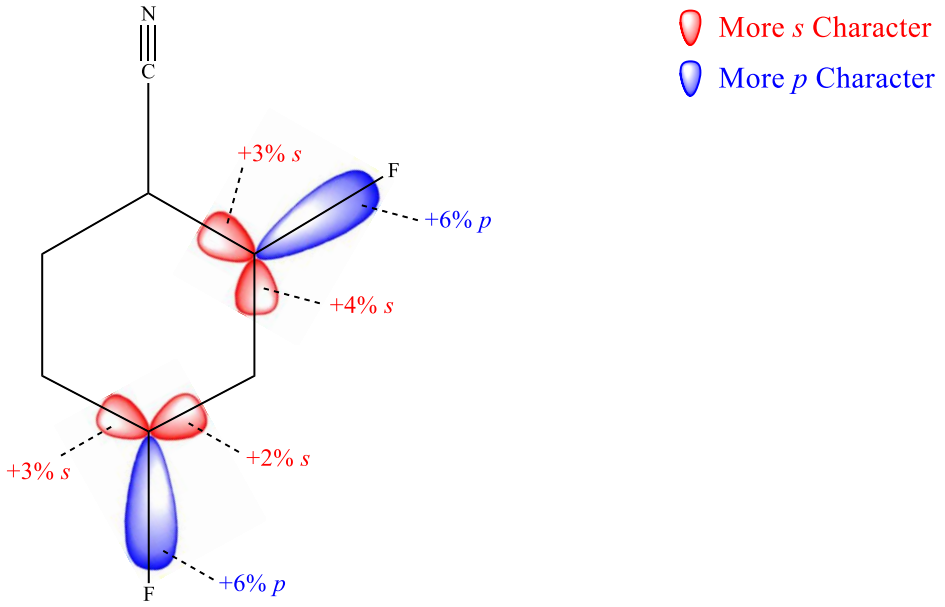


Figure 5.10: Perturbation of hybridization in 24DFBN upon fluorination at the *ortho* and *para* positions according to the NBO analysis results

The distortion of the 24DFBN ring can also be interpreted according to the additivity of effects of the two fluorine atoms. In this molecule, although the fluorine atoms are not in close proximity however, the deformations caused by each fluorine partially overlap with those from another one [9]. According to the δr_0 values, the extent of opening the angles at the fluorination sites is close to that observed in mono-fluorinated BN's. However, while the extent of contraction of the adjacent angles at C1 and C5 are similar to that in 2FBN and 3FBN, the angle at C3 decreases by a greater extent (3.1°). Such a pattern in the angular distortions in 24DFBN can be caused by the superimposition of independent contributions from each fluorine atom as observed in the related fluorinated benzenes including 1,3-difluorobenzene [8]. Although the additivity of effects may be responsible for the angular distortions in 24DFBN, such superimposition effects are not convincing for the bond lengths.

The deviation of the outer ring angle C1−C7−N is another aspect of the geometry deformations in 23DFBN and 24DFBN molecules which is worthwhile to examine. Such deviation in both molecules is shown in Figure 5.11.

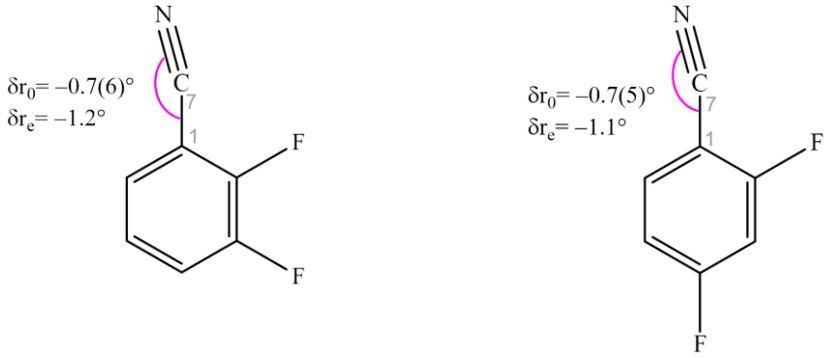


Figure 5.11: Deviation of the C1−C7−N angle from 180° in 23DFBN and 24DFBN, deviations not to scale

According to the δr_0 values, for the C1−C7−N angle in both molecules, a small deviation of 0.7° towards the opposite site of the fluorine atom is observed which is confirmed by the small δr_e value of −1.2°. It is worth noting that the extent of the deviation in the C1−C7−N angle in 23DFBN and 24DFBN is almost the same as that in 2FBN (Chapter 4).

As seen for 2FBN in Chapter 4, the small deviation of the C1−C7−N angle in 23DFBN and 24DFBN molecules can be justified by considering a n→ π* interaction between the lone pairs (n) of electrons on the *ortho*-fluorine atom with the anti-bonding orbital (π*) of the adjacent cyano group. To examine such a n→ π* interaction in 23DFBN and 24DFBN, a natural bonding orbital (NBO) analysis was performed at the MP2/6-311++G(2d,2p) level of theory and all possible interactions between the donor and acceptor NBOs were calculated. It was found that the n→ π* interaction between the non-bonded lone pair (n) on fluorine (donor NBO) with the anti-bonding π* orbital of the C ≡ N bond (acceptor NBO), which is shown in Figure 5.12 and 5.13 for both molecules, is associated with a small stabilization energy of 0.61 kcal.mol^{-1} for 23DFBN and 0.63 kcal.mol^{-1} for 24DFBN which is close to the corresponding value for 2FBN (0.65 kcal.mol^{-1}). Further, according to the calculated natural charges on *ortho*-F and C7 atoms in both molecules, which have opposite signs and almost same values as in 2FBN, one can say that there is an electrostatic contribution to such a non-boding interaction.

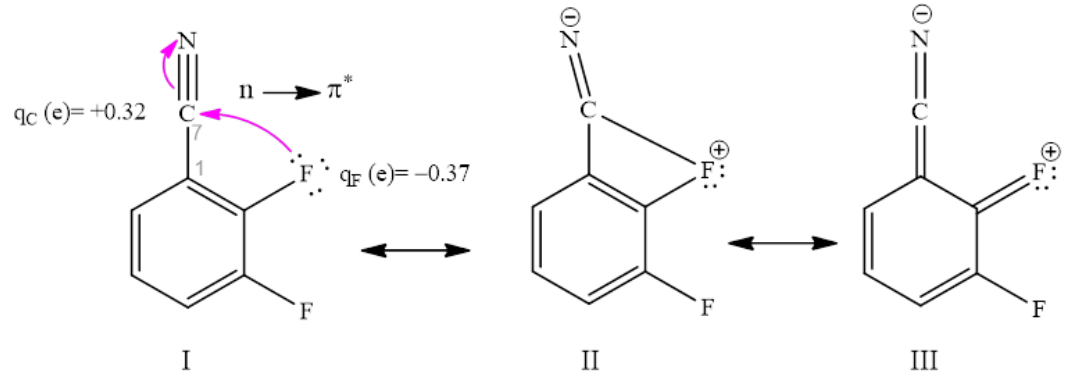


Figure 5.12: The n→ π* interaction between the donor and acceptor NBOs in 23DFBN calculated at the MP2/6-311++G(2d,2p) level along with some possible resonance structures

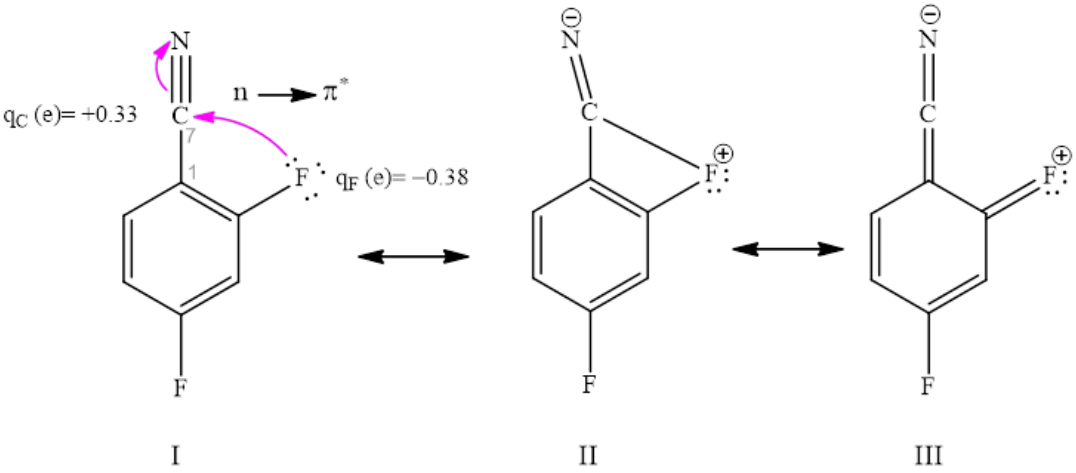


Figure 5.13: The n→ π* interaction between the donor and acceptor NBOs in 24DFBN calculated at the MP2/6-311++G(2d,2p) level along with some possible resonance structures

A four-membered ring (resonance structure II in Figure 5.12 and Figure 5.13) is formed as a result of this n→ π* interaction in which the C1−C7−N angle deviates from 180° towards the opposite of the fluorine atom. The weights of other resonance structures, e.g. resonance form III in Figure 5.12 and Figure 5.13, are likely less important because the aromaticity of ring is broken in them. The resonance form II, will probably have very small weight, however, such a small contribution can be responsible for the observed small deviation of about 1° for the C1−C7−N angle.

It should be mentioned that the calculated value of stabilization energy for the mentioned n→ π* interaction and also the calculated natural charges on *ortho*-F and C7 atoms are almost the same in 23DFBN, 24DFBN and 2FBN molecules which are reflected in the similar extent of deviation in the C1−C7−N angle for these *ortho*-fluorinated compounds.

In summary to this chapter, the results of the MW studies and structural determination for two di-fluorinated derivatives of BN including 23DFBN and 24DFBN were presented. While the substitution (r_s) structures for both molecules could not be accurately determined, a least-squares approach led to more reliable r_0 structures. The observed structural changes based on the r_0 structures, which were supported by the MP2 theory predictions, revealed that in 23DFBN and 24DFBN, most structural deformations happen around the fluorination sites and fewer distortions are seen by going far away from the fluorination sites. While hybridization theory could justify the major deformations in the geometries of the two molecules, the additivity of effects also came into play and could successfully interpret the angular distortions in the ring. It was also found that the *ortho*-fluorinated benzonitriles show a small deviation of about 1° in the outer ring C1−C7−N angle and this deviation was interpreted by considering the role of intramolecular non-bonded n→ π* interactions.

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Chapter 6: Conclusions and future work

In this thesis work, the pure rotational spectra of benzonitrile (BN) and some of its fluorinated derivatives including 2-fluorobenzonitrile (2FBN), 3-fluorobenzonitrile (3FBN), 2,3-difluorobenzonitrile (23DFBN), 2,4-difluorobenzonitrile (24DFBN) and pentafluorobenzonitrile (PFBN) were studied by Fourier transform microwave spectroscopy. The rotational spectra of the studied molecules showed hyperfine splitting arising from the ^{14}N quadrupolar nucleus. Although the microwave spectra of all the parent species were known with the exception of 24DFBN, the microwave spectra of the minor isotopic species, which are vital to evaluate the molecular structure, were mostly unknown and were then investigated in the course of the present study.

Two types of the experimental structures, the substitution (r_s) and effective (r_0) structures, were evaluated for BN and its fluorinated derivatives while the equilibrium (r_e) structures were calculated at the MP2/6-311++G(2d,2p) level of theory. It was found that while the substitution (r_s) structures for these molecules (except for PFBN) could not be accurately determined due to the existence of atoms with the small coordinates in the structure, the effective (r_0) structures were evaluated more reliably.

Using the r_0 and r_e structures, the geometries of fluorinated derivatives were compared to that of the reference compound (BN) and the effect of single, double and full fluorination on the geometry of BN was examined. In partial fluorinated benzonitriles, it was found that the angles at the fluorination sites open by few degrees (2−3°) whereas the adjacent angles reduce by few degrees and also the adjacent C−C bonds contract while the rest of the ring geometry undergo minimal changes. In the fully fluorinated derivative of BN, i.e. in PFBN, it was observed that all the ring bonds shorten and the whole ring is more compact than in BN. Further, most angular deformations in PFBN happened around the cyano substituted carbon

and less distortions were observed in the opposite part of the ring to that point. The variation of the outer ring C7−N bond in the studied molecules was also examined and it was realized that this bond remains unaffected by the fluorination.

To interpret the observed distortions in the BN geometry induced by partial and full fluorination, hybridization theory was successfully used to justify the angular deformations and bond length variations. In the cases of the di-fluorinated benzonitriles, it was found that the additivity of effects can be responsible for the angular distortions although the superimposition effects from the two fluorine atoms were not convincing for the bond lengths. The deviation of the outer ring C1−C7−N angle was also examined and it was found that the *ortho*-fluorinated benzonitriles (2FBN, 23DFBN and 24DFBN) show small deviation of about 1° from 180° in this angle. A natural bonding orbital (NBO) analysis then showed that the non-bonded $n \rightarrow \pi^*$ interaction between the lone pair on fluorine with the anti-bonding π^* orbital of the C ≡ N bond may be responsible for C1−C7−N angle deviation.

In conclusion, it was found that Fourier transform microwave spectroscopy is a valuable technique in evaluating molecular structure. The obtained geometries from this technique have the precision of few thousandths of Ångstroms for bond lengths and few tenths of degrees for bond angles. Such accuracy allows one to track the structural changes induced by a substitution. Further, the good consistency between the structural trends observed from the r_0 structures with those predicted by the MP2 theory can be an important test of the computational chemistry methods.

There are a few points that can be considered to improve the current work. One is to extend the range of spectral measurements to a higher frequency range, e.g. to the millimeter-wave region such that the spectroscopic constants, especially the centrifugal distortion parameters, can be more accurately determined. Another enhancement is to record the rotational

transitions due to the deuterium (^{2}H) substituted isotopologues. Although such extremely weak transitions were not observable in the course of current research due to the very small natural abundance of ^{2}H species, they can be recorded if one synthesizes the deuterium labeled compounds. By including more isotopic data in the least-squares fit, a more accurate effective (r_0) structure may be determined. In addition to microwave spectroscopy, infrared spectroscopy can also be utilized since the analysis of the vibrational spectrum can give information about the molecular structure. For instance, the vibrational analysis of some of the halogenated benzonitriles have been reported in the literature [1-4] from which it was found that the C−H, C−N, C−C and C−X (X=halogen) stretching vibrations are active in the infrared spectrum and therefore, the variation of such vibrations as a function of fluorination can be examined.

Beyond the fluorinated benzonitriles, the chlorinated derivatives of BN can be studied by microwave spectroscopy and by comparing the results with those from the current research, it will be possible to examine the distortion of the benzene ring in BN as a function of the electronegativity and size of the electron-withdrawing atomic substituent. Further, the BN derivatives with electron-donating substituents are other suitable candidates as the deformations induced by such groups are opposite to those induced by the electron-withdrawing substituents, i.e. reducing the angle at the substitution site and elongation of the adjacent bonds and bond angles [5].

In this work, the obtained molecular structures from microwave spectroscopy were good tests of the *ab initio* theory results. In fact, the halogenated benzonitriles are planar molecules and there are not many complications in evaluation of either their experimental or theoretical structures. One can therefore extend the challenge and study the molecules with multiple conformers or with tunneling motions for which the computational chemistry methods are hardly able to predict the stable conformer(s) or to describe the complicated situations in the

molecule. In such cases, the capabilities of the Fourier transform microwave spectroscopy will be good evaluators of the computational chemistry predictions.

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List of Appendices

Appendix I. Microwave transitions of the benzonitrile (BN) and its isotopologues

Table I(A). Microwave transitions of the parent BN in MHz

J'	$K_{a'}$	$K_{c'}$	F'	→	J"	$K_{a"}$	$K_{c"}$	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
2	0	2	2	→	1	0	1	2	5501.92089	-0.00029
2	0	2	1	→	1	0	1	0	5502.12093	-0.00084
2	0	2	2	→	1	0	1	1	5503.19329	0.00108
2	0	2	3	→	1	0	1	2	5503.27626	0.00052
2	0	2	1	→	1	0	1	1	5505.30045	0.00068
2	1	1	2	→	1	1	0	1	5853.96411	-0.00049
2	1	1	2	→	1	1	0	2	5854.54858	-0.00039
2	1	1	1	→	1	1	0	1	5855.10909	-0.00013
2	1	1	3	→	1	1	0	2	5855.28492	0.00050
2	1	1	1	→	1	1	0	0	5856.56992	-0.00050
3	1	3	3	→	2	1	2	3	7772.46301	-0.00074
3	1	3	3	→	2	1	2	2	7773.09034	0.00029
3	1	3	4	→	2	1	2	3	7773.46504	0.00090
3	1	3	2	→	2	1	2	1	7773.46504	-0.00093
3	1	3	2	→	2	1	2	2	7774.44037	-0.00063
3	0	3	3	→	2	0	2	3	8205.43472	-0.00095
3	0	3	2	→	2	0	2	1	8206.56416	-0.00016
3	0	3	3	→	2	0	2	2	8206.78927	-0.00095
3	0	3	4	→	2	0	2	3	8206.83006	0.00080
3	0	3	2	→	2	0	2	2	8208.67197	0.00008
3	2	2	3	→	2	2	1	2	8282.75318	0.00011
3	2	2	4	→	2	2	1	3	8284.11790	0.00304
3	2	2	2	→	2	2	1	1	8284.87078	-0.00099
3	2	1	3	→	2	2	0	2	8359.79777	0.00027
3	2	1	4	→	2	2	0	3	8361.17292	0.00219
3	2	1	2	→	2	2	0	1	8361.92968	-0.00046
3	1	2	3	→	2	1	1	3	8769.05249	-0.00099
3	1	2	3	→	2	1	1	2	8769.78901	0.00008
3	1	2	2	→	2	1	1	1	8770.14650	-0.00111
3	1	2	4	→	2	1	1	3	8770.16731	0.00052
3	1	2	2	→	2	1	1	2	8771.29076	-0.00147
4	1	4	4	→	3	1	3	4	10342.35235	-0.00070
4	1	4	4	→	3	1	3	3	10343.35384	0.00041
4	1	4	3	→	3	1	3	2	10343.46617	-0.00029
4	1	4	5	→	3	1	3	4	10343.51825	0.00091
4	1	4	3	→	3	1	3	3	10344.81675	-0.00066
4	0	4	4	→	3	0	3	4	10853.84908	-0.00077
4	0	4	3	→	3	0	3	2	10855.13575	0.00017
4	0	4	4	→	3	0	3	3	10855.24300	-0.00045
4	0	4	5	→	3	0	3	4	10855.26157	0.00093

4	0	4	3	→	3	0	3	3	10857.01710	-0.00014
4	2	3	4	→	3	2	2	3	11029.57800	0.00030
4	2	3	5	→	3	2	2	4	11030.15428	0.00058
4	2	3	3	→	3	2	2	2	11030.30206	0.00036
4	3	2	4	→	3	3	1	3	11080.79274	0.00046
4	3	2	5	→	3	3	1	4	11082.05603	0.00055
4	3	2	3	→	3	3	1	2	11082.54402	-0.00021
4	3	1	4	→	3	3	0	3	11085.02300	-0.00058
4	3	1	5	→	3	3	0	4	11086.28719	-0.00038
4	3	1	3	→	3	3	0	2	11086.77534	-0.00116
4	2	2	4	→	3	2	1	3	11219.42083	0.00013
4	2	2	5	→	3	2	1	4	11220.01225	0.00063
4	2	2	3	→	3	2	1	2	11220.16172	0.00001
4	1	3	4	→	3	1	2	4	11667.87919	-0.00120
4	1	3	4	→	3	1	2	3	11668.99401	0.00031
4	1	3	3	→	3	1	2	2	11669.09908	0.00057
4	1	3	5	→	3	1	2	4	11669.15974	0.00036
4	1	3	3	→	3	1	2	3	11670.60106	-0.00074
5	1	5	5	→	4	1	4	5	12896.33354	-0.00148
5	1	5	5	→	4	1	4	4	12897.50003	0.00072
5	1	5	4	→	4	1	4	3	12897.54245	0.00040
5	1	5	6	→	4	1	4	5	12897.58714	0.00058
5	1	5	4	→	4	1	4	4	12899.00424	-0.00178
5	0	5	5	→	4	0	4	5	13435.95919	-0.00034
5	0	5	4	→	4	0	4	3	13437.30105	0.00005
5	0	5	5	→	4	0	4	4	13437.36981	-0.00051
5	0	5	6	→	4	0	4	5	13437.37703	0.00162
5	0	5	4	→	4	0	4	4	13439.07385	-0.00095
5	2	4	5	→	4	2	3	5	13762.52239	-0.00057
5	2	4	5	→	4	2	3	4	13763.09922	0.00036
5	2	4	6	→	4	2	3	5	13763.39909	0.00089
5	2	4	4	→	4	2	3	3	13763.42760	-0.00071
5	2	4	4	→	4	2	3	4	13764.15155	-0.00105
5	3	3	5	→	4	3	2	4	13865.27990	0.00033
5	3	3	6	→	4	3	2	5	13865.93472	0.00027
5	3	3	4	→	4	3	2	3	13866.09469	0.00016
5	3	2	5	→	4	3	1	4	13880.02136	0.00037
5	3	2	6	→	4	3	1	5	13880.67813	0.00056
5	3	2	4	→	4	3	1	3	13880.83769	-0.00026
5	2	3	5	→	4	2	2	4	14131.93459	0.00024
5	2	3	6	→	4	2	2	5	14132.25193	0.00112
5	2	3	4	→	4	2	2	3	14132.28143	-0.00119
5	1	4	5	→	4	1	3	4	14545.09292	0.00019
5	1	4	4	→	4	1	3	3	14545.12907	-0.00036
5	1	4	6	→	4	1	3	5	14545.18084	0.00080
6	1	6	6	→	5	1	5	5	15433.91615	0.00019

6	1	6	5	→	5	1	5	4	15433.93287	0.00001
6	1	6	7	→	5	1	5	6	15433.96861	0.00081
6	0	6	6	→	5	0	5	6	15950.52109	-0.00138
6	0	6	5	→	5	0	5	4	15951.88773	0.00028
6	0	6	7	→	5	0	5	6	15951.93817	0.00108
6	0	6	6	→	5	0	5	5	15951.93817	-0.00018
6	0	6	5	→	5	0	5	5	15953.59144	-0.00049
6	2	5	6	→	5	2	4	5	16480.52213	0.00020
6	2	5	5	→	5	2	4	4	16480.69764	0.00074
6	2	5	7	→	5	2	4	6	16480.69764	0.00006
6	4	3	6	→	5	4	2	5	16632.59567	0.00093
6	4	3	7	→	5	4	2	6	16633.26618	0.00074
6	4	2	6	→	5	4	1	5	16633.36210	0.00045
6	4	3	5	→	5	4	2	4	16633.40944	0.00024
6	4	2	7	→	5	4	1	6	16634.03228	-0.00017
6	4	2	5	→	5	4	1	4	16634.17441	-0.00181
6	3	4	6	→	5	3	3	5	16655.05920	-0.00045
6	3	4	7	→	5	3	3	6	16655.44579	0.00103
6	3	4	5	→	5	3	3	4	16655.50318	-0.00117
6	3	3	6	→	5	3	2	5	16694.03638	0.00031
6	3	3	7	→	5	3	2	6	16694.42515	0.00084
6	3	3	5	→	5	3	2	4	16694.48277	-0.00154
6	2	4	6	→	5	2	3	5	17095.45670	-0.00048
6	2	4	7	→	5	2	3	6	17095.65044	0.00027
6	2	4	5	→	5	2	3	4	17095.65044	0.00004
6	1	5	6	→	5	1	4	5	17389.72912	-0.00118
6	1	5	5	→	5	1	4	4	17389.74344	0.00236
6	1	5	7	→	5	1	4	6	17389.78014	-0.00018
7	1	7	7	→	6	1	6	6	17952.15764	-0.00064
7	1	7	6	→	6	1	6	5	17952.16499	0.00105
7	1	7	8	→	6	1	6	7	17952.19187	0.00060
7	0	7	6	→	6	0	6	5	18409.34944	-0.00013
7	0	7	8	→	6	0	6	7	18409.38466	0.00013
7	0	7	7	→	6	0	6	6	18409.38888	0.00044
7	2	6	7	→	6	2	5	6	19179.00150	-0.00032
7	2	6	6	→	6	2	5	5	19179.10125	-0.00162
7	2	6	8	→	6	2	5	7	19179.11520	0.00228
7	4	4	7	→	6	4	3	6	19423.84769	0.00049
7	4	4	8	→	6	4	3	7	19424.27501	-0.00012
7	4	4	6	→	6	4	3	5	19424.34352	0.00166
7	4	3	7	→	6	4	2	6	19426.39269	-0.00011
7	4	3	8	→	6	4	2	7	19426.81990	-0.00107
7	4	3	6	→	6	4	2	5	19426.88779	0.00007
7	3	5	7	→	6	3	4	6	19448.33987	0.00079
7	3	5	8	→	6	3	4	7	19448.58664	0.00113
7	3	5	6	→	6	3	4	5	19448.60569	-0.00202

7	3	4	7	→	6	3	3	6	19534.78566	0.00033
7	3	4	8	→	6	3	3	7	19535.03756	0.00083
7	3	4	6	→	6	3	3	5	19535.05774	-0.00178
7	2	5	7	→	6	2	4	6	20095.96507	0.00042
7	2	5	6	→	6	2	4	5	20096.08049	-0.00202
7	2	5	8	→	6	2	4	7	20096.09270	0.00096
7	1	6	6	→	6	1	5	5	20192.93425	0.00144
7	1	6	7	→	6	1	5	6	20192.93425	-0.00025
7	1	6	8	→	6	1	5	7	20192.96341	-0.00008
8	1	8	8	→	7	1	7	7	20452.90380	0.00009
8	1	8	7	→	7	1	7	6	20452.90380	-0.00025
8	1	8	9	→	7	1	7	8	20452.92552	-0.00022
8	0	8	7	→	7	0	7	6	20828.17622	0.00075
8	0	8	9	→	7	0	7	8	20828.20297	0.00089
8	0	8	8	→	7	0	7	7	20828.20297	-0.00242
8	2	7	8	→	7	2	6	7	21855.93236	-0.00013
8	2	7	7	→	7	2	6	6	21855.99398	-0.00079
8	2	7	9	→	7	2	6	8	21856.00780	0.00107
8	4	5	8	→	7	4	4	7	22222.94934	0.00059
8	4	5	9	→	7	4	4	8	22223.24063	0.00133
8	4	5	7	→	7	4	4	6	22223.27036	-0.00141
8	4	4	8	→	7	4	3	7	22229.90336	-0.00021
8	4	4	9	→	7	4	3	8	22230.19557	0.00096
8	4	4	7	→	7	4	3	6	22230.22476	-0.00239
8	3	6	8	→	7	3	5	7	22242.07854	-0.00094
8	3	6	9	→	7	3	5	8	22242.24589	-0.00094
8	3	6	7	→	7	3	5	6	22242.25520	0.00172
8	3	5	8	→	7	3	4	7	22411.09040	-0.00008
8	3	5	9	→	7	3	4	8	22411.26446	-0.00063
8	3	5	7	→	7	3	4	6	22411.27378	0.00132
9	1	9	8	→	8	1	8	7	22937.73301	0.00143
9	1	9	9	→	8	1	8	8	22937.73301	-0.00085
9	1	9	10	→	8	1	8	9	22937.74935	0.00022
8	1	7	7	→	7	1	6	6	22943.46284	-0.00165
8	1	7	8	→	7	1	6	7	22943.47459	0.00113
8	1	7	9	→	7	1	6	8	22943.48982	0.00081
8	2	6	8	→	7	2	5	7	23110.91624	-0.00116
8	2	6	7	→	7	2	5	6	23110.99118	-0.00145
8	2	6	9	→	7	2	5	8	23111.00725	0.00275
9	0	9	8	→	8	0	8	7	23227.69141	-0.00023
9	0	9	10	→	8	0	8	9	23227.71275	0.00091
9	0	9	9	→	8	0	8	8	23227.71275	-0.00129
9	2	8	9	→	8	2	7	8	24509.13783	0.00079
9	2	8	8	→	8	2	7	7	24509.17383	-0.00275
9	2	8	10	→	8	2	7	9	24509.18966	0.00129

Table I(B). Microwave transitions of the $^{13}C_1$ isotopologue of BN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
3	1	3	3	→	2	1	2	2	7767.53194	-0.00088
3	1	3	4	→	2	1	2	3	7767.90660	-0.00008
3	1	3	2	→	2	1	2	1	7767.90660	-0.00046
3	0	3	2	→	2	0	2	1	8200.44665	-0.00178
3	0	3	3	→	2	0	2	2	8200.67258	-0.00011
3	0	3	4	→	2	0	2	3	8200.71308	0.00044
4	1	4	4	→	3	1	3	3	10336.01313	0.00065
4	1	4	3	→	3	1	3	2	10336.12513	0.00002
4	1	4	5	→	3	1	3	4	10336.17616	-0.00039
4	0	4	3	→	3	0	3	2	10847.26719	-0.00086
4	0	4	4	→	3	0	3	3	10847.37283	-0.00139
4	0	4	5	→	3	0	3	4	10847.39367	0.00099
4	2	3	4	→	3	2	2	3	11021.12569	0.00012
4	2	3	5	→	3	2	2	4	11021.70104	0.00042
4	2	3	3	→	3	2	2	2	11021.84781	-0.00057
4	2	2	4	→	3	2	1	3	11210.33038	-0.00104
4	2	2	5	→	3	2	1	4	11210.92039	0.00033
4	2	2	3	→	3	2	1	2	11211.06796	-0.00177
4	1	3	4	→	3	1	2	3	11659.59000	0.00028
4	1	3	3	→	3	1	2	2	11659.69562	0.00033
4	1	3	5	→	3	1	2	4	11659.75544	0.00018
5	1	5	5	→	4	1	4	4	12888.42646	0.00266
5	1	5	4	→	4	1	4	3	12888.46641	-0.00017
5	1	5	6	→	4	1	4	5	12888.51087	-0.00051
5	0	5	4	→	4	0	4	3	13427.87122	-0.00114
5	0	5	5	→	4	0	4	4	13427.94005	0.00017
5	0	5	6	→	4	0	4	5	13427.94727	0.00080
6	0	6	5	→	5	0	5	4	15941.04414	0.00057
6	0	6	7	→	5	0	5	6	15941.09272	-0.00028
6	0	6	6	→	5	0	5	5	15941.09272	0.00006
6	2	5	6	→	5	2	4	5	16468.06374	0.00146
6	2	5	5	→	5	2	4	4	16468.23681	-0.00048
6	2	5	7	→	5	2	4	6	16468.23681	-0.00111
6	2	4	6	→	5	2	3	5	17081.08834	-0.00004
6	2	4	7	→	5	2	3	6	17081.28078	0.00104
6	2	4	5	→	5	2	3	4	17081.28078	0.00088
6	1	5	6	→	5	1	4	5	17376.04657	0.00019
6	1	5	5	→	5	1	4	4	17376.06012	0.00207
6	1	5	7	→	5	1	4	6	17376.09739	0.00053
7	0	7	6	→	6	0	6	5	18397.14668	0.00050
7	0	7	8	→	6	0	6	7	18397.18208	0.00109
7	0	7	7	→	6	0	6	6	18397.18208	-0.00128

7	1	6	6	→	6	1	5	5	20177.33386	0.00045
7	1	6	7	→	6	1	5	6	20177.33386	-0.00020
7	1	6	8	→	6	1	5	7	20177.36111	-0.00264
8	1	8	8	→	7	1	7	7	20438.90184	0.00122
8	1	8	7	→	7	1	7	6	20438.90184	0.00050
8	1	8	9	→	7	1	7	8	20438.92148	-0.00163
8	0	8	7	→	7	0	7	6	20814.57981	0.00134
8	0	8	9	→	7	0	7	8	20814.60481	-0.00020
8	0	8	8	→	7	0	7	7	20814.60481	-0.00214

Table I(C). Microwave transitions of the $^{13}C_2$ isotopologue of BN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
3	1	3	3	→	2	1	2	2	7753.01982	0.00066
3	1	3	4	→	2	1	2	3	7753.39425	-0.00013
3	1	3	2	→	2	1	2	1	7753.39425	-0.00011
3	0	3	2	→	2	0	2	1	8189.77812	-0.00143
3	0	3	3	→	2	0	2	2	8190.00433	-0.00064
3	0	3	4	→	2	0	2	3	8190.04464	-0.00013
4	1	4	4	→	3	1	3	3	10315.65142	0.00080
4	1	4	3	→	3	1	3	2	10315.76344	0.00000
4	1	4	5	→	3	1	3	4	10315.81517	-0.00008
4	0	4	3	→	3	0	3	2	10828.84974	-0.00080
4	0	4	4	→	3	0	3	3	10828.95658	-0.00088
4	0	4	5	→	3	0	3	4	10828.97677	0.00111
4	2	3	4	→	3	2	2	3	11011.31532	0.00128
4	2	3	5	→	3	2	2	4	11011.89114	0.00002
4	2	3	3	→	3	2	2	2	11012.03942	0.00003
4	2	2	4	→	3	2	1	3	11209.89231	-0.00104
4	2	2	5	→	3	2	1	4	11210.48439	0.00000
4	2	2	3	→	3	2	1	2	11210.63412	-0.00050
4	1	3	4	→	3	1	2	3	11657.90626	0.00029
4	1	3	3	→	3	1	2	2	11658.01226	0.00037
4	1	3	5	→	3	1	2	4	11658.07207	0.00014
5	1	5	5	→	4	1	4	4	12861.51827	-0.00029
5	1	5	4	→	4	1	4	3	12861.56127	-0.00005
5	1	5	6	→	4	1	4	5	12861.60570	-0.00070
5	0	5	4	→	4	0	4	3	13399.09330	-0.00117
5	0	5	5	→	4	0	4	4	13399.16231	-0.00019
5	0	5	6	→	4	0	4	5	13399.16909	0.00023
5	2	4	5	→	4	2	3	4	13739.12438	0.00007
5	2	4	6	→	4	2	3	5	13739.42393	-0.00039
5	2	4	4	→	4	2	3	3	13739.45405	-0.00046
6	1	6	6	→	5	1	5	5	15389.02799	0.00012
6	1	6	5	→	5	1	5	4	15389.04786	0.00293
6	1	6	7	→	5	1	5	6	15389.07993	-0.00031
6	0	6	5	→	5	0	5	4	15900.21397	-0.00154
6	0	6	7	→	5	0	5	6	15900.26533	0.00024
6	0	6	6	→	5	0	5	5	15900.26533	0.00052
6	2	5	6	→	5	2	4	5	16450.09135	0.00037
6	2	5	5	→	5	2	4	4	16450.26705	0.00076
6	2	5	7	→	5	2	4	6	16450.26705	-0.00002
6	2	4	6	→	5	2	3	5	17090.28536	-0.00090
6	2	4	7	→	5	2	3	6	17090.47936	0.00111
6	2	4	5	→	5	2	3	4	17090.47936	0.00099

6	1	5	6	→	5	1	4	5	17367.08444	-0.00062
6	1	5	5	→	5	1	4	4	17367.09883	0.00254
6	1	5	7	→	5	1	4	6	17367.13523	-0.00019
7	1	7	7	→	6	1	6	6	17897.82807	-0.00023
7	1	7	6	→	6	1	6	5	17897.83521	0.00099
7	1	7	8	→	6	1	6	7	17897.86127	-0.00055
7	0	7	6	→	6	0	6	5	18344.17796	0.00094
7	0	7	8	→	6	0	6	7	18344.21269	0.00059
7	0	7	7	→	6	0	6	6	18344.21269	-0.00147
7	1	6	6	→	6	1	5	5	20161.27502	-0.00103
7	1	6	7	→	6	1	5	6	20161.27502	-0.00183
7	1	6	8	→	6	1	5	7	20161.30703	0.00076
8	1	8	8	→	7	1	7	7	20388.74895	0.00110
8	1	8	7	→	7	1	7	6	20388.74895	0.00044
8	1	8	9	→	7	1	7	8	20388.76834	-0.00207
8	0	8	7	→	7	0	7	6	20750.79632	0.00182
8	0	8	9	→	7	0	7	8	20750.82075	-0.00010
8	0	8	8	→	7	0	7	7	20750.82075	-0.00178
8	2	7	8	→	7	2	6	7	21809.91686	-0.00142
8	2	7	7	→	7	2	6	6	21809.97886	-0.00216
8	2	7	9	→	7	2	6	8	21809.99588	0.00291

Table I(D). Microwave transitions of the $^{13}C_3$ isotopologue of BN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
3	1	3	3	→	2	1	2	2	7706.50277	0.00147
3	1	3	4	→	2	1	2	3	7706.87541	-0.00118
3	1	3	2	→	2	1	2	1	7706.87541	-0.00101
3	0	3	2	→	2	0	2	1	8138.62225	-0.00096
3	0	3	3	→	2	0	2	2	8138.84784	-0.00035
3	0	3	4	→	2	0	2	3	8138.88794	-0.00040
4	1	4	4	→	3	1	3	3	10254.22180	-0.00022
4	1	4	3	→	3	1	3	2	10254.33562	0.00074
4	1	4	5	→	3	1	3	4	10254.38641	-0.00035
4	0	4	3	→	3	0	3	2	10763.10878	-0.00043
4	0	4	4	→	3	0	3	3	10763.21347	-0.00216
4	0	4	5	→	3	0	3	4	10763.23404	-0.00023
4	2	3	4	→	3	2	2	3	10940.53196	-0.00010
4	2	3	5	→	3	2	2	4	10941.10918	0.00004
4	2	3	3	→	3	2	2	2	10941.25642	-0.00100
4	2	2	4	→	3	2	1	3	11133.62615	-0.00042
4	2	2	5	→	3	2	1	4	11134.21751	0.00033
4	2	2	3	→	3	2	1	2	11134.36836	0.00101
4	1	3	4	→	3	1	2	3	11579.18200	0.00072
4	1	3	3	→	3	1	2	2	11579.28782	0.00041
4	1	3	5	→	3	1	2	4	11579.34751	0.00018
5	1	5	5	→	4	1	4	4	12785.59894	0.00079
5	1	5	4	→	4	1	4	3	12785.64220	0.00120
5	1	5	6	→	4	1	4	5	12785.68518	-0.00093
5	0	5	4	→	4	0	4	3	13320.37840	-0.00067
5	0	5	5	→	4	0	4	4	13320.44712	0.00052
5	0	5	6	→	4	0	4	5	13320.45388	0.00047
5	2	4	5	→	4	2	3	4	13651.36130	-0.00014
5	2	4	6	→	4	2	3	5	13651.66179	0.00027
5	2	4	4	→	4	2	3	3	13651.69132	-0.00040
6	1	6	6	→	5	1	5	5	15299.03755	-0.00056
6	1	6	5	→	5	1	5	4	15299.05853	0.00324
6	1	6	7	→	5	1	5	6	15299.08941	-0.00121
6	0	6	5	→	5	0	5	4	15809.72397	0.00051
6	0	6	7	→	5	0	5	6	15809.77272	-0.00031
6	0	6	6	→	5	0	5	5	15809.77272	0.00036
6	2	5	6	→	5	2	4	5	16345.81124	-0.00257
6	2	5	5	→	5	2	4	4	16345.99064	0.00135
6	2	5	7	→	5	2	4	6	16345.99064	0.00061
6	2	4	6	→	5	2	3	5	16969.71003	0.00029
6	2	4	7	→	5	2	3	6	16969.90264	0.00119
6	2	4	5	→	5	2	3	4	16969.90264	0.00106

6	1	5	6	→	5	1	4	5	17252.66063	-0.00100
6	1	5	5	→	5	1	4	4	17252.67480	0.00141
6	1	5	7	→	5	1	4	6	17252.71216	-0.00008
7	1	7	7	→	6	1	6	6	17794.14895	-0.00045
7	1	7	6	→	6	1	6	5	17794.15614	0.00070
7	1	7	8	→	6	1	6	7	17794.18220	-0.00085
7	0	7	6	→	6	0	6	5	18242.31615	0.00051
7	0	7	8	→	6	0	6	7	18242.35212	0.00144
7	0	7	7	→	6	0	6	6	18242.35212	-0.00039
7	1	6	6	→	6	1	5	5	20030.94690	0.00200
7	1	6	7	→	6	1	5	6	20030.94690	0.00138
7	1	6	8	→	6	1	5	7	20030.97242	-0.00285
8	1	8	8	→	7	1	7	7	20271.68465	0.00109
8	1	8	7	→	7	1	7	6	20271.68465	0.00033
8	1	8	9	→	7	1	7	8	20271.70336	-0.00287
8	0	8	7	→	7	0	7	6	20637.22212	0.00185
8	0	8	9	→	7	0	7	8	20637.24700	0.00031
8	0	8	8	→	7	0	7	7	20637.24700	-0.00121
8	2	7	8	→	7	2	6	7	21674.29855	0.00107
8	2	7	7	→	7	2	6	6	21674.35864	-0.00174
8	2	7	9	→	7	2	6	8	21674.37330	0.00099

Table I(E). Microwave transitions of the $^{13}C_4$ isotopologue of BN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
3	1	3	3	→	2	1	2	2	7674.36272	0.00162
3	1	3	4	→	2	1	2	3	7674.73543	0.00044
3	1	3	2	→	2	1	2	1	7674.73543	-0.00026
3	0	3	2	→	2	0	2	1	8098.21626	-0.00007
3	0	3	3	→	2	0	2	2	8098.44066	0.00033
3	0	3	4	→	2	0	2	3	8098.48067	0.00015
4	1	4	4	→	3	1	3	3	10212.86333	0.00029
4	1	4	3	→	3	1	3	2	10212.97526	-0.00061
4	1	4	5	→	3	1	3	4	10213.02709	-0.00007
4	0	4	3	→	3	0	3	2	10715.43869	-0.00049
4	0	4	4	→	3	0	3	3	10715.54336	-0.00170
4	0	4	5	→	3	0	3	4	10715.56483	0.00103
4	1	3	4	→	3	1	2	3	11503.36993	0.00051
4	1	3	3	→	3	1	2	2	11503.47478	-0.00022
4	1	3	5	→	3	1	2	4	11503.53459	-0.00052
5	1	5	5	→	4	1	4	4	12736.06523	0.00107
5	1	5	4	→	4	1	4	3	12736.10667	-0.00041
5	1	5	6	→	4	1	4	5	12736.15072	-0.00107
5	0	5	4	→	4	0	4	3	13269.44320	-0.00097
5	0	5	5	→	4	0	4	4	13269.51133	-0.00015
5	0	5	6	→	4	0	4	5	13269.51940	0.00111
6	0	6	5	→	5	0	5	4	15758.36232	0.00033
6	0	6	7	→	5	0	5	6	15758.41136	-0.00009
6	0	6	6	→	5	0	5	5	15758.41136	0.00032
6	2	5	6	→	5	2	4	5	16260.04991	-0.00147
6	2	5	5	→	5	2	4	4	16260.22710	0.00228
6	2	5	7	→	5	2	4	6	16260.22710	0.00061
6	2	4	6	→	5	2	3	5	16843.19829	-0.00109
6	2	4	7	→	5	2	3	6	16843.39180	0.00102
6	2	4	5	→	5	2	3	4	16843.39180	0.00082
6	1	5	6	→	5	1	4	5	17148.25698	-0.00107
6	1	5	5	→	5	1	4	4	17148.27058	0.00066
6	1	5	7	→	5	1	4	6	17148.31003	0.00126
7	0	7	6	→	6	0	6	5	18191.18241	-0.00110
7	0	7	8	→	6	0	6	7	18191.22111	0.00108
7	0	7	7	→	6	0	6	6	18191.22111	-0.00039
7	1	6	6	→	6	1	5	5	19917.21490	0.00153
7	1	6	7	→	6	1	5	6	19917.21490	0.00116
7	1	6	8	→	6	1	5	7	19917.24208	-0.00165
8	0	8	7	→	7	0	7	6	20584.90421	0.00043
8	0	8	9	→	7	0	7	8	20584.93038	0.00168
8	0	8	8	→	7	0	7	7	20584.93038	-0.00162

Table I(F). Microwave transitions of the $^{13}C_5$ isotopologue of BN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
3	1	3	3	→	2	1	2	2	7695.55421	0.00036
3	1	3	4	→	2	1	2	3	7695.92851	-0.00007
3	1	3	2	→	2	1	2	1	7695.92851	-0.00085
3	0	3	2	→	2	0	2	1	8121.48378	0.00026
3	0	3	3	→	2	0	2	2	8121.70796	-0.00028
3	0	3	4	→	2	0	2	3	8121.74858	0.00021
4	1	4	4	→	3	1	3	3	10240.87531	-0.00055
4	1	4	3	→	3	1	3	2	10240.98975	0.00082
4	1	4	5	→	3	1	3	4	10241.04028	-0.00002
4	0	4	3	→	3	0	3	2	10745.44539	-0.00138
4	0	4	4	→	3	0	3	3	10745.55141	-0.00172
4	0	4	5	→	3	0	3	4	10745.57161	-0.00010
4	1	3	4	→	3	1	2	3	11538.93345	0.00129
4	1	3	3	→	3	1	2	2	11539.03884	0.00095
4	1	3	5	→	3	1	2	4	11539.09743	-0.00077
5	1	5	5	→	4	1	4	4	12770.72554	0.00321
5	1	5	4	→	4	1	4	3	12770.76441	-0.00089
5	1	5	6	→	4	1	4	5	12770.81077	0.00067
5	0	5	4	→	4	0	4	3	13305.50761	-0.00110
5	0	5	5	→	4	0	4	4	13305.57626	-0.00014
5	0	5	6	→	4	0	4	5	13305.58355	0.00053
6	0	6	5	→	5	0	5	4	15799.94217	-0.00065
6	0	6	7	→	5	0	5	6	15799.99222	-0.00018
6	0	6	6	→	5	0	5	5	15799.99222	0.00005
6	2	5	6	→	5	2	4	5	16307.36884	0.00012
6	2	5	7	→	5	2	4	6	16307.48891	-0.00008
6	2	5	5	→	5	2	4	4	16307.56373	-0.00008
6	2	4	6	→	5	2	3	5	16897.32358	-0.00154
6	2	4	7	→	5	2	3	6	16897.51757	0.00047
6	2	4	5	→	5	2	3	4	16897.51757	0.00027
6	1	5	6	→	5	1	4	5	17200.12382	-0.00140
6	1	5	5	→	5	1	4	4	17200.13849	0.00150
6	1	5	7	→	5	1	4	6	17200.17651	0.00056
7	1	6	6	→	6	1	5	5	19976.45517	0.00155
7	1	6	7	→	6	1	5	6	19976.45517	0.00101
7	1	6	8	→	6	1	5	7	19976.48320	-0.00088
8	1	8	8	→	7	1	7	7	20256.87590	-0.00040
8	1	8	7	→	7	1	7	6	20256.87590	-0.00107
8	1	8	9	→	7	1	7	8	20256.89944	0.00063

Table I(G). Microwave transitions of the ^{15}N isotopologue of BN in MHz

J'	K_a'	K_c'	→	J"	K_a"	K_c"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
3	1	3	→	2	1	2	7582.65378	0.00072
3	0	3	→	2	0	2	7997.56680	0.00000
3	1	2	→	2	1	1	8528.52026	0.00029
4	1	4	→	3	1	3	10091.35830	-0.00053
4	0	4	→	3	0	3	10585.28146	-0.00028
4	2	3	→	3	2	2	10741.72851	-0.00013
4	2	2	→	3	2	1	10911.65024	-0.00058
4	1	3	→	3	1	2	11349.74648	0.00017
5	1	5	→	4	1	4	12585.60000	0.00031
5	0	5	→	4	0	4	13112.73331	-0.00025
5	2	4	→	4	2	3	13405.55576	0.00042

Appendix II. Microwave transitions of the pentafluorobenzonitrile (PFBN) and its isotopologues

Table II(A). Microwave transitions of the parent PFBN in MHz

J'	K_a'	K_c'	F'	→	J"	K_a"	K_c"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	2	3	4	→	3	2	2	3	4671.92765	0.00007
4	2	3	5	→	3	2	2	4	4672.44356	0.00025
4	2	3	3	→	3	2	2	2	4672.57536	-0.00030
5	1	5	5	→	4	1	4	4	4823.99137	0.00007
5	1	5	4	→	4	1	4	3	4824.01090	-0.00083
5	1	5	6	→	4	1	4	5	4824.05585	-0.00030
5	0	5	4	→	4	0	4	3	4829.62069	0.00052
5	0	5	5	→	4	0	4	4	4829.62069	-0.00031
5	0	5	6	→	4	0	4	5	4829.66858	-0.00056
4	1	3	3	→	3	1	2	2	4940.95145	0.00020
4	1	3	5	→	3	1	2	4	4941.06410	-0.00022
4	1	3	4	→	3	1	2	3	4941.15057	0.00051
4	3	2	4	→	3	3	1	3	5035.38026	-0.00009
4	3	2	5	→	3	3	1	4	5036.73750	-0.00017
4	3	2	3	→	3	3	1	2	5037.25063	0.00006
4	3	1	4	→	3	3	0	3	5336.02951	-0.00035
4	3	1	5	→	3	3	0	4	5337.59558	-0.00035
4	3	1	3	→	3	3	0	2	5338.15059	-0.00067
4	2	2	4	→	3	2	1	3	5503.09106	-0.00001
4	2	2	5	→	3	2	1	4	5503.57191	-0.00001
4	2	2	3	→	3	2	1	2	5503.65874	0.00043
6	1	6	6	→	5	1	5	5	5703.29101	0.00036
6	1	6	5	→	5	1	5	4	5703.30316	0.00036
6	1	6	7	→	5	1	5	6	5703.33489	-0.00028
6	0	6	6	→	5	0	5	5	5704.48221	-0.00096
6	0	6	5	→	5	0	5	4	5704.49338	0.00165
6	0	6	7	→	5	0	5	6	5704.52464	-0.00010
5	1	4	4	→	4	1	3	3	5780.23580	-0.00008
5	1	4	6	→	4	1	3	5	5780.29456	-0.00001
5	1	4	5	→	4	1	3	4	5780.34753	-0.00039
5	3	3	5	→	4	3	2	4	6215.05208	-0.00026
5	3	3	6	→	4	3	2	5	6215.67991	-0.00018
5	3	3	4	→	4	3	2	3	6215.82908	-0.00028
5	4	2	5	→	4	4	1	4	6382.96519	-0.00007
5	4	2	6	→	4	4	1	5	6384.24565	0.00123
5	4	2	4	→	4	4	1	3	6384.61335	0.00055
5	4	1	5	→	4	4	0	4	6519.22599	0.00062
5	4	1	6	→	4	4	0	5	6520.63652	0.00131
5	4	1	4	→	4	4	0	3	6521.02899	0.00071
6	2	5	6	→	5	2	4	5	6567.35890	-0.00019

6	2	5	5	→	5	2	4	4	6567.45807	-0.00213
6	2	5	7	→	5	2	4	6	6567.46838	0.00087
7	1	7	7	→	6	1	6	6	6581.03548	-0.00086
7	1	7	6	→	6	1	6	5	6581.04712	0.00127
7	1	7	8	→	6	1	6	7	6581.07007	-0.00014
7	0	7	7	→	6	0	6	6	6581.27006	-0.00154
7	0	7	6	→	6	0	6	5	6581.28209	0.00156
7	0	7	8	→	6	0	6	7	6581.30477	-0.00021
6	1	5	6	→	5	1	4	5	6611.10749	0.00032
6	1	5	5	→	5	1	4	4	6611.10749	0.00068
6	1	5	7	→	5	1	4	6	6611.13147	-0.00054
5	2	3	5	→	4	2	2	4	6699.79627	0.00041
5	2	3	4	→	4	2	2	3	6699.82016	-0.00146
5	2	3	6	→	4	2	2	5	6699.85613	-0.00021
5	3	2	5	→	4	3	1	4	6882.38697	-0.00023
5	3	2	6	→	4	3	1	5	6883.12615	-0.00001
5	3	2	4	→	4	3	1	3	6883.28018	-0.00025
6	3	4	6	→	5	3	3	5	7295.18294	0.00004
6	3	4	7	→	5	3	3	6	7295.48122	0.00005
6	3	4	5	→	5	3	3	4	7295.52316	-0.00045
7	2	6	7	→	6	2	5	6	7457.36018	0.00007
7	2	6	6	→	6	2	5	5	7457.41784	-0.00110
7	2	6	8	→	6	2	5	7	7457.43037	0.00050
8	1	8	8	→	7	1	7	7	7458.47669	-0.00026
8	1	8	7	→	7	1	7	6	7458.48604	0.00114
8	1	8	9	→	7	1	7	8	7458.50411	0.00021
8	0	8	8	→	7	0	7	7	7458.52064	-0.00058
8	0	8	7	→	7	0	7	6	7458.53073	0.00166
8	0	8	9	→	7	0	7	8	7458.54787	-0.00021
7	1	6	7	→	6	1	5	6	7469.12434	-0.00051
7	1	6	6	→	6	1	5	5	7469.16042	0.00067
7	1	6	8	→	6	1	5	7	7469.17376	-0.00027
6	2	4	5	→	5	2	3	4	7648.30989	0.00021
6	2	4	7	→	5	2	3	6	7648.36007	0.00007
6	2	4	6	→	5	2	3	5	7648.46422	0.00018
6	4	3	6	→	5	4	2	5	7659.48619	0.00017
6	4	3	7	→	5	4	2	6	7660.18736	0.00032
6	4	3	5	→	5	4	2	4	7660.33078	-0.00010
6	5	2	6	→	5	5	1	5	7682.48507	-0.00043
6	5	2	7	→	5	5	1	6	7683.66912	0.00032
6	5	2	5	→	5	5	1	4	7683.94543	-0.00014
6	5	1	6	→	5	5	0	5	7732.52508	0.00011
6	5	1	7	→	5	5	0	6	7733.76051	0.00012
6	5	1	5	→	5	5	0	4	7734.04531	-0.00032
6	4	2	6	→	5	4	1	5	8092.30629	-0.00018
6	4	2	7	→	5	4	1	6	8093.19318	0.00019

6	4	2	5	→	5	4	1	4	8093.36212	-0.00003
7	3	5	7	→	6	3	4	6	8281.70416	0.00004
7	3	5	8	→	6	3	4	7	8281.84833	-0.00070
7	3	5	6	→	6	3	4	5	8281.85845	0.00146
6	3	3	6	→	5	3	2	5	8292.56267	-0.00006
6	3	3	7	→	5	3	2	6	8292.83084	0.00061
6	3	3	5	→	5	3	2	4	8292.85077	-0.00132
8	2	7	8	→	7	2	6	7	8337.51463	-0.00005
8	2	7	7	→	7	2	6	6	8337.55664	-0.00138
8	2	7	9	→	7	2	6	8	8337.56851	0.00057
8	1	7	8	→	7	1	6	7	8340.31344	-0.00028
8	1	7	7	→	7	1	6	6	8340.35156	-0.00041
8	1	7	9	→	7	1	6	8	8340.36300	0.00039
7	2	5	6	→	6	2	4	5	8452.48681	0.00027
7	2	5	8	→	6	2	4	7	8452.51660	0.00011
7	2	5	7	→	6	2	4	6	8452.58184	0.00020
7	4	4	7	→	6	4	3	6	8851.90947	-0.00010
7	4	4	8	→	6	4	3	7	8852.29103	0.00034
7	4	4	6	→	6	4	3	5	8852.34619	-0.00019
7	6	2	7	→	6	6	1	6	8959.23363	0.00090
7	6	2	8	→	6	6	1	7	8960.31831	0.00092
7	6	2	6	→	6	6	1	5	8960.53228	0.00057
7	6	1	7	→	6	6	0	6	8975.36775	0.00097
7	6	1	8	→	6	6	0	7	8976.46942	0.00124
7	6	1	6	→	6	6	0	5	8976.68531	0.00045
7	5	3	7	→	6	5	2	6	9021.10906	-0.00027
7	5	3	8	→	6	5	2	7	9021.84481	0.00038
7	5	3	6	→	6	5	2	5	9021.97507	-0.00041
8	3	6	8	→	7	3	5	7	9204.34000	-0.00012
8	3	6	7	→	7	3	5	6	9204.41960	0.00148
8	3	6	9	→	7	3	5	8	9204.41960	-0.00069
10	0	10	10	→	9	0	9	9	9213.28333	-0.00178
10	1	10	10	→	9	1	9	9	9213.28333	-0.00035
10	0	10	9	→	9	0	9	8	9213.29177	0.00091
10	1	10	9	→	9	1	9	8	9213.29177	0.00233
10	0	10	11	→	9	0	9	10	9213.30264	-0.00074
10	1	10	11	→	9	1	9	10	9213.30264	0.00068
9	2	8	9	→	8	2	7	8	9215.08290	0.00000
9	2	8	8	→	8	2	7	7	9215.11682	-0.00133
9	2	8	10	→	8	2	7	9	9215.12797	0.00106
9	1	8	9	→	8	1	7	8	9215.69803	-0.00018
9	1	8	8	→	8	1	7	7	9215.73137	-0.00109
9	1	8	10	→	8	1	7	9	9215.74257	0.00123
7	5	2	7	→	6	5	1	6	9238.14538	-0.00024
7	5	2	8	→	6	5	1	7	9239.01627	-0.00009
7	5	2	6	→	6	5	1	5	9239.16527	-0.00018

8	2	6	7	→	7	2	5	6	9264.24022	-0.00148
8	2	6	8	→	7	2	5	7	9264.24887	-0.00026
8	2	6	9	→	7	2	5	8	9264.25613	0.00106
7	3	4	6	→	6	3	3	5	9457.28402	0.00062
7	3	4	8	→	6	3	3	7	9457.30634	-0.00081
7	3	4	7	→	6	3	3	6	9457.31291	0.00048
7	4	3	7	→	6	4	2	6	9682.49373	-0.00020
7	4	3	8	→	6	4	2	7	9682.97290	0.00024
7	4	3	6	→	6	4	2	5	9683.03354	-0.00022
8	4	5	8	→	7	4	4	7	9937.57541	0.00022
8	4	5	9	→	7	4	4	8	9937.77375	0.00055
8	4	5	7	→	7	4	4	6	9937.79103	-0.00066
11	0	11	11	→	10	0	10	10	10090.69809	-0.00087
11	1	11	11	→	10	1	10	10	10090.69809	-0.00062
11	0	11	10	→	10	0	10	9	10090.70411	0.00020
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11	1	11	12	→	10	1	10	11	10090.71485	0.00071
10	2	9	10	→	9	2	8	9	10092.18461	0.00031
10	2	9	9	→	9	2	8	8	10092.21274	-0.00126
10	2	9	11	→	9	2	8	10	10092.22186	0.00021
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10	1	9	9	→	9	1	8	8	10092.34044	-0.00127
10	1	9	11	→	9	1	8	10	10092.34963	0.00025
9	3	7	9	→	8	3	6	8	10095.43130	0.00053
9	3	7	8	→	8	3	6	7	10095.48050	-0.00153
9	3	7	10	→	8	3	6	9	10095.48722	0.00081
9	2	7	9	→	8	2	6	8	10112.74472	-0.00017
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9	2	7	10	→	8	2	6	9	10112.78110	0.00118
8	7	2	8	→	7	7	1	7	10227.54077	-0.00017
8	7	2	9	→	7	7	1	8	10228.53474	0.00014
8	7	2	7	→	7	7	1	6	10228.70425	-0.00059
8	7	1	8	→	7	7	0	7	10232.32737	-0.00027
8	7	1	9	→	7	7	0	8	10233.32615	0.00006
8	7	1	7	→	7	7	0	6	10233.49634	-0.00059
8	5	4	8	→	7	5	3	7	10311.09431	0.00007
8	5	4	9	→	7	5	3	8	10311.54674	0.00035
8	5	4	7	→	7	5	3	6	10311.60819	-0.00028
8	6	3	8	→	7	6	2	7	10327.21700	0.00005
8	6	3	9	→	7	6	2	8	10327.95222	0.00049
8	6	3	7	→	7	6	2	6	10328.06717	-0.00017
8	3	5	7	→	7	3	4	6	10355.58640	0.00062
8	3	5	9	→	7	3	4	8	10355.61714	-0.00009
8	3	5	8	→	7	3	4	7	10355.73222	0.00011
8	6	2	8	→	7	6	1	7	10415.51427	0.00002

8	6	2	9	→	7	6	1	8	10416.31249	0.00011
8	6	2	7	→	7	6	1	6	10416.43560	-0.00002
8	5	3	8	→	7	5	2	7	10880.05545	-0.00019
8	5	3	9	→	7	5	2	8	10880.67677	-0.00032
8	5	3	7	→	7	5	2	6	10880.75719	0.00032
9	4	6	9	→	8	4	5	8	10925.82478	-0.00004
9	4	6	10	→	8	4	5	9	10925.92604	-0.00007
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12	1	12	12	→	11	1	11	11	10968.11912	-0.00132
12	0	12	11	→	11	0	11	10	10968.12471	-0.00007
12	1	12	11	→	11	1	11	10	10968.12471	-0.00003
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10	3	8	10	→	9	3	7	9	10975.08127	0.00011
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10	2	8	10	→	9	2	7	9	10979.53036	0.00046
10	2	8	9	→	9	2	7	8	10979.56471	-0.00085
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8	4	4	8	→	7	4	3	7	11090.45612	0.00027
8	4	4	9	→	7	4	3	8	11090.62032	-0.00081
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9	3	6	8	→	8	3	5	7	11126.32414	-0.00002
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9	8	2	9	→	8	8	1	8	11493.51371	0.00066
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11	3	9	11	→	10	3	8	10	11851.72957	-0.00068
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10	3	7	11	→	9	3	6	10	11920.89017	-0.00022
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9	6	3	9	→	8	6	2	8	11990.78389	-0.00030
9	6	3	10	→	8	6	2	9	11991.42195	0.00010
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9	4	5	8	→	8	4	4	7	12213.65763	-0.00034
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9	5	4	9	→	8	5	3	8	12498.83111	-0.00007
9	5	4	10	→	8	5	3	9	12499.17806	0.00078
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10	5	6	10	→	9	5	5	9	12593.00874	-0.00065
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13	2	12	13	→	12	2	11	12	12723.73683	0.00055
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12	3	10	12	→	11	3	9	11	12727.98633	0.00105
12	3	10	11	→	11	3	9	10	12728.01639	-0.00103
12	3	10	13	→	11	3	9	12	12728.02147	0.00022
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11	4	8	11	→	10	4	7	10	12738.31941	0.00015
11	4	8	10	→	10	4	7	9	12738.36072	0.00189
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11	3	8	11	→	10	3	7	10	12760.32064	0.00016
11	3	8	10	→	10	3	7	9	12760.33766	-0.00071
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10	8	3	11	→	9	8	2	10	12870.10838	0.00037
10	8	3	9	→	9	8	2	8	12870.19449	-0.00044
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10	6	5	11	→	9	6	4	10	12981.52612	0.00067
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13	3	11	13	→	12	3	10	12	13604.43047	0.00071

13	3	11	12	→	12	3	10	11	13604.45744	-0.00110
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16	1	16	16	→	15	1	15	15	14477.83926	-0.00008
16	1	16	15	→	15	1	15	14	14477.83926	-0.00270
16	0	16	17	→	15	0	15	16	14477.84804	0.00092
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15	1	14	15	→	14	1	13	14	14478.36620	-0.00083
15	2	14	15	→	14	2	13	14	14478.36620	-0.00080

15	1	14	14	→	14	1	13	13	14478.38043	-0.00141
15	2	14	14	→	14	2	13	13	14478.38043	-0.00138
15	2	14	16	→	14	2	13	15	14478.38716	0.00109
15	1	14	16	→	14	1	13	15	14478.38716	0.00106
14	3	12	14	→	13	3	11	13	14481.11208	0.00041
14	2	12	14	→	13	2	11	13	14481.12282	0.00074
14	3	12	13	→	13	3	11	12	14481.13571	-0.00179
14	3	12	15	→	13	3	11	14	14481.13986	-0.00088
14	2	12	13	→	13	2	11	12	14481.14731	-0.00059
14	2	12	15	→	13	2	11	14	14481.15148	0.00034
13	4	10	13	→	12	4	9	12	14491.37380	0.00042
13	4	10	12	→	12	4	9	11	14491.40576	0.00098
13	4	10	14	→	12	4	9	13	14491.40576	-0.00145
13	3	10	13	→	12	3	9	12	14492.87397	0.00052
13	3	10	12	→	12	3	9	11	14492.90466	0.00118
13	3	10	14	→	12	3	9	13	14492.90466	-0.00141
12	5	8	12	→	11	5	7	11	14498.37004	0.00032
12	5	8	11	→	11	5	7	10	14498.41067	0.00027
12	5	8	13	→	11	5	7	12	14498.41067	-0.00117
12	4	8	11	→	11	4	7	10	14580.41965	-0.00142
12	4	8	13	→	11	4	7	12	14580.42850	0.00054
12	4	8	12	→	11	4	7	11	14580.44368	0.00017
12	6	7	12	→	11	6	6	11	15257.86669	-0.00057
12	6	7	13	→	11	6	6	12	15257.97067	-0.00076
12	6	7	11	→	11	6	6	10	15257.97693	0.00058
11	6	5	11	→	10	6	4	10	15325.61790	0.00019
11	6	5	12	→	10	6	4	11	15325.88069	-0.00041
11	6	5	10	→	10	6	4	9	15325.89993	0.00109
17	0	17	17	→	16	0	16	16	15355.27307	0.00060
17	0	17	16	→	16	0	16	15	15355.27307	-0.00174
17	1	17	17	→	16	1	16	16	15355.27307	0.00060
17	1	17	16	→	16	1	16	15	15355.27307	-0.00174
17	0	17	18	→	16	0	16	17	15355.28024	0.00082
17	1	17	18	→	16	1	16	17	15355.28024	0.00082
16	1	15	16	→	15	1	14	15	15355.71972	-0.00168
16	2	15	16	→	15	2	14	15	15355.71972	-0.00167
16	1	15	15	→	15	1	14	14	15355.73408	-0.00049
16	2	15	15	→	15	2	14	14	15355.73408	-0.00049
16	1	15	17	→	15	1	14	16	15355.73950	0.00107
16	2	15	17	→	15	2	14	16	15355.73950	0.00108
15	3	13	15	→	14	3	12	14	15357.98133	0.00227
15	2	13	15	→	14	2	12	14	15357.98133	0.00019
15	3	13	14	→	14	3	12	13	15358.00425	0.00196
15	2	13	14	→	14	2	12	13	15358.00425	-0.00012
15	3	13	16	→	14	3	12	15	15358.00750	0.00221
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14	4	11	14	→	13	4	10	13	15366.28992	0.00019
14	4	11	13	→	13	4	10	12	15366.31862	-0.00046
14	4	11	15	→	13	4	10	14	15366.32141	0.00004
14	3	11	14	→	13	3	10	13	15366.64497	0.00012
14	3	11	13	→	13	3	10	12	15366.67359	-0.00031
14	3	11	15	→	13	3	10	14	15366.67629	0.00008
13	5	9	13	→	12	5	8	12	15385.61596	0.00054
13	5	9	12	→	12	5	8	11	15385.64583	0.00097
13	5	9	14	→	12	5	8	13	15385.64583	-0.00106
12	10	3	12	→	11	10	2	11	15393.22027	0.00084
12	10	3	13	→	11	10	2	12	15393.83476	-0.00052
12	10	3	11	→	11	10	2	10	15393.90479	0.00351
12	10	2	12	→	11	10	1	11	15394.10957	-0.00136
12	10	2	13	→	11	10	1	12	15394.72456	-0.00285
12	10	2	11	→	11	10	1	10	15394.79400	0.00053
13	4	9	13	→	12	4	8	12	15411.41050	-0.00147
13	4	9	12	→	12	4	8	11	15411.42157	0.00001
13	4	9	14	→	12	4	8	13	15411.42633	0.00116
12	9	4	12	→	11	9	3	11	15531.47157	-0.00007
12	9	4	13	→	11	9	3	12	15531.98258	0.00004
12	9	4	11	→	11	9	3	10	15532.03326	-0.00034
12	9	3	12	→	11	9	2	11	15549.28656	-0.00017
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12	9	3	11	→	11	9	2	10	15549.86542	-0.00051
12	7	6	12	→	11	7	5	11	15664.62395	-0.00033
12	7	6	13	→	11	7	5	12	15664.87136	-0.00008
12	7	6	11	→	11	7	5	10	15664.89065	-0.00035
12	8	5	12	→	11	8	4	11	15679.21189	-0.00006
12	8	5	13	→	11	8	4	12	15679.61007	0.00033
12	8	5	11	→	11	8	4	10	15679.64551	-0.00074
12	5	7	11	→	11	5	6	10	15763.83348	-0.00011
12	5	7	13	→	11	5	6	12	15763.85057	-0.00015
12	5	7	12	→	11	5	6	11	15763.97152	0.00000
12	8	4	12	→	11	8	3	11	15869.03652	-0.00001
12	8	4	13	→	11	8	3	12	15869.51479	0.00054
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17	1	16	17	→	16	1	15	16	16233.09144	-0.00084
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17	1	16	16	→	16	1	15	15	16233.10348	-0.00060
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17	1	16	18	→	16	1	15	17	16233.10808	0.00050
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16	3	14	16	→	15	3	13	15	16234.98009	0.00040
16	3	14	16	→	15	3	13	15	16234.98009	0.00040
16	3	14	15	→	15	3	13	14	16235.00055	-0.00010
16	3	14	15	→	15	3	13	14	16235.00055	-0.00010
16	3	14	17	→	15	3	13	16	16235.00406	0.00064
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13	6	8	13	→	12	6	7	12	16238.07679	-0.00029
13	6	8	14	→	12	6	7	13	16238.13008	-0.00007
13	6	8	12	→	12	6	7	11	16238.13008	-0.00030
15	4	12	15	→	14	4	11	14	16241.68533	0.00082
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15	3	12	16	→	14	3	11	15	16241.79217	-0.00199
14	5	10	14	→	13	5	9	13	16261.13528	0.00056
14	5	10	13	→	13	5	9	12	16261.16216	0.00081
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12	7	5	12	→	11	7	4	11	16518.94703	-0.00004
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12	6	6	12	→	11	6	5	11	16692.93960	-0.00105
12	6	6	11	→	11	6	5	10	16693.00011	0.00201
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13	10	4	13	→	12	10	3	12	16788.04816	0.00030
13	10	4	14	→	12	10	3	13	16788.54384	0.00070
13	10	4	12	→	12	10	3	11	16788.58932	-0.00026
13	10	3	13	→	12	10	2	12	16793.81941	-0.00006
13	10	3	14	→	12	10	2	13	16794.31869	0.00059
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13	7	7	13	→	12	7	6	12	16856.95315	-0.00026
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13	7	7	12	→	12	7	6	11	16857.11142	0.00079
13	9	5	13	→	12	9	4	12	16953.95894	-0.00029
13	9	5	14	→	12	9	4	13	16954.36611	0.00004
13	9	5	12	→	12	9	4	11	16954.40135	-0.00032
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13	8	6	13	→	12	8	5	12	17057.77711	0.00001
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19	0	19	19	→	18	0	18	18	17110.13984	0.00016
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19	0	19	20	→	18	0	18	19	17110.14564	0.00031
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17	3	15	17	→	16	3	14	16	17112.07491	-0.00067
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17	3	15	16	→	16	3	14	15	17112.09474	0.00019
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17	3	15	18	→	16	3	14	17	17112.09751	0.00038
17	2	15	18	→	16	2	14	17	17112.09751	0.00030
15	5	11	15	→	14	5	10	14	17134.02701	0.00019
15	5	11	14	→	14	5	10	13	17134.05362	0.00088
15	5	11	16	→	14	5	10	15	17134.05362	-0.00092
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14	6	9	13	→	13	6	8	12	17153.30142	0.00067
14	6	9	15	→	13	6	8	14	17153.30142	-0.00076
14	5	9	13	→	13	5	8	12	17242.32931	-0.00105
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13	8	5	13	→	12	8	4	12	17572.12376	-0.00043
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14	13	2	15	→	13	13	1	14	17825.22315	0.00044
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14	7	8	14	→	13	7	7	13	17929.78299	-0.00059
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19	1	18	20	→	18	1	17	19	17987.88041	0.00055
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18	2	16	18	→	17	2	15	17	17989.24000	-0.00070
18	3	16	18	→	17	3	15	17	17989.24000	-0.00068
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16	5	12	16	→	15	5	11	15	18007.19057	-0.00028
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16	5	12	17	→	15	5	11	16	18007.21709	-0.00065
16	4	12	16	→	15	4	11	15	18007.66555	-0.00019
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15	6	10	15	→	14	6	9	14	18036.79956	-0.00153
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13	7	6	13	→	12	7	5	12	18158.94681	-0.00010
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14	9	6	14	→	13	9	5	13	18377.59645	-0.00025
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20	1	19	20	→	19	1	18	19	18865.26551	-0.00068
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19	3	17	20	→	18	3	16	19	18866.47551	0.00048
18	4	15	18	→	17	4	14	17	18870.28958	-0.00019
18	3	15	18	→	17	3	14	17	18870.28958	-0.00095
18	4	15	17	→	17	4	14	16	18870.31327	0.00185
18	3	15	17	→	17	3	14	16	18870.31327	0.00110
18	4	15	19	→	17	4	14	18	18870.31327	0.00008
18	3	15	19	→	17	3	14	18	18870.31327	-0.00068
17	5	13	17	→	16	5	12	16	18881.19920	0.00007
17	5	13	16	→	16	5	12	15	18881.22483	0.00128
17	5	13	18	→	16	5	12	17	18881.22483	-0.00017
17	4	13	17	→	16	4	12	16	18881.31072	-0.00066
17	4	13	16	→	16	4	12	15	18881.33666	0.00093
17	4	13	18	→	16	4	12	17	18881.33666	-0.00052
15	7	9	15	→	14	7	8	14	18902.78975	0.00112
15	7	9	14	→	14	7	8	13	18902.82711	0.00009
15	7	9	16	→	14	7	8	15	18902.82711	-0.00028
16	6	11	16	→	15	6	10	15	18909.21928	-0.00163
16	6	11	15	→	15	6	10	14	18909.24229	0.00102

16	6	11	17	→	15	6	10	16	18909.24229	-0.00055
16	5	11	16	→	15	5	10	15	18917.63342	-0.00066
16	5	11	15	→	15	5	10	14	18917.65104	0.00183
16	5	11	17	→	15	5	10	16	18917.65104	-0.00008
15	6	9	14	→	14	6	8	13	19151.55851	-0.00164
15	6	9	16	→	14	6	8	15	19151.56997	0.00115
15	6	9	15	→	14	6	8	14	19151.64137	0.00024
14	8	6	14	→	13	8	5	13	19360.69375	-0.00014
14	8	6	15	→	13	8	5	14	19361.02020	-0.00028
14	8	6	13	→	13	8	5	12	19361.04136	0.00039
14	7	7	14	→	13	7	6	13	19491.91973	0.00021
14	7	7	13	→	13	7	6	12	19491.94323	0.00009
14	7	7	15	→	13	7	6	14	19491.94687	0.00021
15	8	8	15	→	14	8	7	14	19543.53243	0.00045
15	8	8	16	→	14	8	7	15	19543.64808	-0.00059
15	8	8	14	→	14	8	7	13	19543.65490	0.00063
15	10	6	15	→	14	10	5	14	19651.40319	0.00017
15	10	6	16	→	14	10	5	15	19651.73533	0.00017
15	10	6	14	→	14	10	5	13	19651.75960	0.00054
22	0	22	22	→	21	0	21	21	19742.44052	0.00072
22	1	22	22	→	21	1	21	21	19742.44052	0.00072
22	0	22	21	→	21	0	21	20	19742.44052	-0.00075
22	1	22	21	→	21	1	21	20	19742.44052	-0.00075
22	0	22	23	→	21	0	21	22	19742.44427	0.00019
22	1	22	23	→	21	1	21	22	19742.44427	0.00019
20	2	18	20	→	19	2	17	19	19743.71114	-0.00107
20	3	18	20	→	19	3	17	19	19743.71114	-0.00107
20	2	18	19	→	19	2	17	18	19743.72886	0.00227
20	3	18	19	→	19	3	17	18	19743.72886	0.00227
20	2	18	21	→	19	2	17	20	19743.72886	0.00019
20	3	18	21	→	19	3	17	20	19743.72886	0.00019
19	4	16	19	→	18	4	15	18	19746.98310	-0.00055
19	3	16	19	→	18	3	15	18	19746.98310	-0.00070
19	4	16	18	→	18	4	15	17	19747.00545	0.00180
19	3	16	18	→	18	3	15	17	19747.00545	0.00164
19	4	16	20	→	18	4	15	19	19747.00545	0.00012
19	3	16	20	→	18	3	15	19	19747.00545	-0.00003
17	5	12	17	→	16	5	11	16	19781.83489	-0.00088
17	5	12	16	→	16	5	11	15	19781.85630	0.00103
17	5	12	18	→	16	5	11	17	19781.85630	-0.00042
15	7	8	14	→	14	7	7	13	20456.79004	-0.00104
15	7	8	16	→	14	7	7	15	20456.80330	0.00104
15	7	8	15	→	14	7	7	14	20456.89722	-0.00026
16	8	9	16	→	15	8	8	15	20607.10866	0.00080
16	8	9	17	→	15	8	8	16	20607.16884	0.00064
16	8	9	15	→	15	8	8	14	20607.16884	-0.00073

21	2	19	21	→	20	2	18	20	20620.99600	-0.00107
21	3	19	21	→	20	3	18	20	20620.99600	-0.00107
21	2	19	20	→	20	2	18	19	20621.01254	0.00227
21	3	19	20	→	20	3	18	19	20621.01254	0.00227
21	2	19	22	→	20	2	18	21	20621.01254	0.00032
21	3	19	22	→	20	3	18	21	20621.01254	0.00032
20	3	17	20	→	19	3	16	19	20623.81892	-0.00192
20	4	17	20	→	19	4	16	19	20623.81892	-0.00189
20	4	17	19	→	19	4	16	18	20623.84133	0.00201
20	3	17	19	→	19	3	16	18	20623.84133	0.00198
20	4	17	21	→	19	4	16	20	20623.84133	0.00042
20	3	17	21	→	19	3	16	20	20623.84133	0.00039
18	6	13	18	→	17	6	12	17	20650.62922	-0.00155
18	6	13	17	→	17	6	12	16	20650.65330	0.00126
18	6	13	19	→	17	6	12	18	20650.65330	0.00006
18	5	13	18	→	17	5	12	17	20651.21810	-0.00114
18	5	13	17	→	17	5	12	16	20651.24154	0.00138
18	5	13	19	→	17	5	12	18	20651.24154	0.00016
17	7	11	17	→	16	7	10	16	20691.37642	-0.00140
17	7	11	16	→	16	7	10	15	20691.39447	0.00172
17	7	11	18	→	16	7	10	17	20691.39447	0.00019
15	8	7	15	→	14	8	6	14	20995.88685	0.00001
15	8	7	16	→	14	8	6	15	20996.04784	-0.00025
15	8	7	14	→	14	8	6	13	20996.05567	0.00086
16	9	8	16	→	15	9	7	15	21059.15328	-0.00009
16	9	8	17	→	15	9	7	16	21059.31240	0.00002
16	9	8	15	→	15	9	7	14	21059.32200	0.00113
16	7	9	15	→	15	7	8	14	21159.84361	-0.00053
16	7	9	17	→	15	7	8	16	21159.85640	0.00109
16	7	9	16	→	15	7	8	15	21159.97219	-0.00033
11	7	4	10	→	10	5	5	9	21494.20286	0.00083
11	7	4	12	→	10	5	5	11	21494.26612	-0.00004
11	7	4	11	→	10	5	5	10	21494.86832	-0.00124
23	1	22	23	→	22	1	21	22	21497.48842	-0.00077
23	2	22	23	→	22	2	21	22	21497.48842	-0.00077
23	1	22	22	→	22	1	21	21	21497.49816	0.00225
23	2	22	22	→	22	2	21	21	21497.49816	0.00225
23	1	22	24	→	22	1	21	23	21497.49816	0.00013
23	2	22	24	→	22	2	21	23	21497.49816	0.00013
22	2	20	22	→	21	2	19	21	21498.30379	-0.00128
22	3	20	22	→	21	3	19	21	21498.30379	-0.00128
22	2	20	21	→	21	2	19	20	21498.31919	0.00196
22	3	20	21	→	21	3	19	20	21498.31919	0.00196
22	2	20	23	→	21	2	19	22	21498.31919	0.00014
22	3	20	23	→	21	3	19	22	21498.31919	0.00014
21	3	18	21	→	20	3	17	20	21500.76512	-0.00094

21	4	18	21	→	20	4	17	20	21500.76512	-0.00094
21	3	18	20	→	20	3	17	19	21500.78530	0.00209
21	4	18	20	→	20	4	17	19	21500.78530	0.00210
21	3	18	22	→	20	3	17	21	21500.78530	0.00059
21	4	18	22	→	20	4	17	21	21500.78530	0.00059
19	6	14	19	→	18	6	13	18	21522.97309	-0.00102
19	6	14	18	→	18	6	13	17	21522.99666	0.00135
19	6	14	20	→	18	6	13	19	21522.99666	0.00026
19	5	14	19	→	18	5	13	18	21523.11768	-0.00086
19	5	14	18	→	18	5	13	17	21523.14114	0.00149
19	5	14	20	→	18	5	13	19	21523.14114	0.00039
18	7	12	18	→	17	7	11	17	21560.27000	-0.00187
18	7	12	17	→	17	7	11	16	21560.28856	0.00151
18	7	12	19	→	17	7	11	18	21560.28856	0.00015
18	6	12	18	→	17	6	11	17	21569.57626	-0.00076
18	6	12	17	→	17	6	11	16	21569.58918	0.00187
18	6	12	19	→	17	6	11	18	21569.58918	0.00026
17	8	10	17	→	16	8	9	16	21571.67727	0.00020
17	8	10	16	→	16	8	9	15	21571.70518	0.00076
17	8	10	18	→	16	8	9	17	21571.70518	0.00007
17	7	10	16	→	16	7	9	15	21826.82494	-0.00154
17	7	10	18	→	16	7	9	17	21826.83447	0.00101
17	7	10	17	→	16	7	9	16	21826.90456	0.00101

Table II(B). Microwave transitions of the $^{13}C_1$ isotopologue of PFBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
7	1	7	7	→	6	1	6	6	6572.87141	-0.00108
7	1	7	6	→	6	1	6	5	6572.88381	0.00181
7	1	7	8	→	6	1	6	7	6572.90640	-0.00004
7	0	7	7	→	6	0	6	6	6573.11622	-0.00131
7	0	7	6	→	6	0	6	5	6573.12774	0.00132
7	0	7	8	→	6	0	6	7	6573.15080	-0.00016
6	1	5	5	→	5	1	4	4	6603.58584	0.00066
6	1	5	6	→	5	1	4	5	6603.58584	-0.00049
6	1	5	7	→	5	1	4	6	6603.60975	-0.00087
7	2	6	7	→	6	2	5	6	7447.99523	0.00011
7	2	6	6	→	6	2	5	5	7448.05283	-0.00135
7	2	6	8	→	6	2	5	7	7448.06546	0.00030
8	1	8	8	→	7	1	7	7	7449.22654	-0.00041
8	1	8	7	→	7	1	7	6	7449.23774	0.00285
8	1	8	9	→	7	1	7	8	7449.25436	0.00041
8	0	8	8	→	7	0	7	7	7449.27220	-0.00119
8	0	8	7	→	7	0	7	6	7449.28278	0.00155
8	0	8	9	→	7	0	7	8	7449.30006	-0.00024
6	2	4	5	→	5	2	3	4	7639.91464	0.00133
6	2	4	7	→	5	2	3	6	7639.96338	0.00003
6	2	4	6	→	5	2	3	5	7640.06492	-0.00014
7	3	5	7	→	6	3	4	6	8269.93371	-0.00025
7	3	5	8	→	6	3	4	7	8270.07935	-0.00068
7	3	5	6	→	6	3	4	5	8270.08889	0.00077
7	2	5	6	→	6	2	4	5	8444.11823	-0.00044
7	2	5	8	→	6	2	4	7	8444.14818	-0.00065
7	2	5	7	→	6	2	4	6	8444.21490	0.00037
10	0	10	10	→	9	0	9	9	9201.85500	-0.00286
10	1	10	10	→	9	1	9	9	9201.85500	-0.00134
10	0	10	9	→	9	0	9	8	9201.86383	0.00022
10	1	10	9	→	9	1	9	8	9201.86383	0.00174
10	0	10	11	→	9	0	9	10	9201.87586	-0.00031
10	1	10	11	→	9	1	9	10	9201.87586	0.00120
9	2	8	9	→	8	2	7	8	9203.67078	-0.00031
9	2	8	8	→	8	2	7	7	9203.70466	-0.00172
9	2	8	10	→	8	2	7	9	9203.71634	0.00117
11	0	11	11	→	10	0	10	10	10078.18231	-0.00054
11	1	11	11	→	10	1	10	10	10078.18231	-0.00027
11	0	11	10	→	10	0	10	9	10078.18986	0.00206
11	1	11	10	→	10	1	10	9	10078.18986	0.00233
11	0	11	12	→	10	0	10	11	10078.19715	-0.00116
11	1	11	12	→	10	1	10	11	10078.19715	-0.00089

10	2	9	10	→	9	2	8	9	10079.68711	0.00112
10	2	9	9	→	9	2	8	8	10079.71423	-0.00148
10	2	9	11	→	9	2	8	10	10079.72370	0.00031
10	1	9	10	→	9	1	8	9	10079.82237	0.00131
10	1	9	9	→	9	1	8	8	10079.84926	-0.00133
10	1	9	11	→	9	1	8	10	10079.85901	0.00071
9	3	7	9	→	8	3	6	8	10082.79825	0.00056
9	3	7	8	→	8	3	6	7	10082.84740	-0.00178
9	3	7	10	→	8	3	6	9	10082.85439	0.00080
9	2	7	9	→	8	2	6	8	10100.77823	0.00035
9	2	7	8	→	8	2	6	7	10100.80395	-0.00144
9	2	7	10	→	8	2	6	9	10100.81410	0.00152
12	0	12	12	→	11	0	11	11	10954.51334	-0.00233
12	1	12	12	→	11	1	11	11	10954.51334	-0.00229
12	0	12	11	→	11	0	11	10	10954.51977	-0.00019
12	1	12	11	→	11	1	11	10	10954.51977	-0.00015
12	0	12	13	→	11	0	11	12	10954.53024	0.00135
12	1	12	13	→	11	1	11	12	10954.53024	0.00139
10	2	8	10	→	9	2	7	9	10966.17193	0.00076
10	2	8	9	→	9	2	7	8	10966.20558	-0.00112
10	2	8	11	→	9	2	7	10	10966.21267	0.00084
13	0	13	13	→	12	0	12	12	11830.85211	-0.00114
13	1	13	13	→	12	1	12	12	11830.85211	-0.00113
13	0	13	12	→	12	0	12	11	11830.85644	-0.00057
13	1	13	12	→	12	1	12	11	11830.85644	-0.00056
13	0	13	14	→	12	0	12	13	11830.86577	0.00108
13	1	13	14	→	12	1	12	13	11830.86577	0.00109
14	0	14	14	→	13	0	13	13	12707.19422	0.00033
14	0	14	13	→	13	0	13	12	12707.19422	-0.00298
14	1	14	14	→	13	1	13	13	12707.19422	0.00033
14	1	14	13	→	13	1	13	12	12707.19422	-0.00298
14	0	14	15	→	13	0	13	14	12707.20518	0.00130
14	1	14	15	→	13	1	13	14	12707.20518	0.00130
15	0	15	15	→	14	0	14	14	13583.53735	0.00082
15	0	15	14	→	14	0	14	13	13583.53735	-0.00211
15	1	15	15	→	14	1	14	14	13583.53735	0.00082
15	1	15	14	→	14	1	14	13	13583.53735	-0.00211
15	0	15	16	→	14	0	14	15	13583.54661	0.00129
15	1	15	16	→	14	1	14	15	13583.54661	0.00129

Table II(C). Microwave transitions of the $^{13}C_2$ isotopologue of PFBN in MHz

J'	$K_{a'}$	$K_{c'}$	F'	→	J"	$K_{a"}$	$K_{c"}$	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
5	0	5	4	→	4	0	4	3	4822.58537	-0.00022
5	0	5	5	→	4	0	4	4	4822.58537	-0.00073
5	0	5	6	→	4	0	4	5	4822.63369	-0.00060
7	1	7	7	→	6	1	6	6	6571.58864	-0.00170
7	1	7	6	→	6	1	6	5	6571.60014	0.00027
7	1	7	8	→	6	1	6	7	6571.62377	-0.00035
7	0	7	7	→	6	0	6	6	6571.81212	-0.00198
7	0	7	6	→	6	0	6	5	6571.82388	0.00082
7	0	7	8	→	6	0	6	7	6571.84724	-0.00017
6	1	5	5	→	5	1	4	4	6600.84231	-0.00079
6	1	5	6	→	5	1	4	5	6600.84231	-0.00016
6	1	5	7	→	5	1	4	6	6600.86741	-0.00059
5	2	3	5	→	4	2	2	4	6692.70937	-0.00009
5	2	3	4	→	4	2	2	3	6692.72858	-0.00114
5	2	3	6	→	4	2	2	5	6692.76582	0.00043
6	3	4	6	→	5	3	3	5	7287.87056	0.00039
6	3	4	7	→	5	3	3	6	7288.16683	0.00028
6	3	4	5	→	5	3	3	4	7288.20807	-0.00060
7	2	6	7	→	6	2	5	6	7446.77983	-0.00021
7	2	6	6	→	6	2	5	5	7446.83786	-0.00075
7	2	6	8	→	6	2	5	7	7446.84984	0.00036
8	1	8	8	→	7	1	7	7	7447.76872	-0.00050
8	1	8	7	→	7	1	7	6	7447.77830	0.00112
8	1	8	9	→	7	1	7	8	7447.79629	0.00019
8	0	8	8	→	7	0	7	7	7447.81392	0.00296
8	0	8	7	→	7	0	7	6	7447.82175	0.00292
8	0	8	9	→	7	0	7	8	7447.83741	-0.00035
6	2	4	5	→	5	2	3	4	7636.00826	-0.00038
6	2	4	7	→	5	2	3	6	7636.05975	0.00051
6	2	4	6	→	5	2	3	5	7636.16582	0.00005
7	3	5	7	→	6	3	4	6	8271.50771	-0.00054
7	3	5	8	→	6	3	4	7	8271.65107	-0.00071
7	3	5	6	→	6	3	4	5	8271.66104	0.00145
6	3	3	6	→	5	3	2	5	8288.09480	0.00011
6	3	3	7	→	5	3	2	6	8288.35862	0.00090
6	3	3	5	→	5	3	2	4	8288.37801	-0.00067
7	2	5	6	→	6	2	4	5	8437.91703	0.00040
7	2	5	8	→	6	2	4	7	8437.94681	0.00051
7	2	5	7	→	6	2	4	6	8438.01039	-0.00029
10	0	10	10	→	9	0	9	9	9200.05747	-0.00208
10	1	10	10	→	9	1	9	9	9200.05747	-0.00075
10	0	10	9	→	9	0	9	8	9200.06595	0.00065

10	1	10	9	→	9	1	9	8	9200.06595	0.00197
10	0	10	11	→	9	0	9	10	9200.07653	-0.00124
10	1	10	11	→	9	1	9	10	9200.07653	0.00008
9	2	8	9	→	8	2	7	8	9201.83086	0.00024
9	2	8	8	→	8	2	7	7	9201.86370	-0.00213
9	2	8	10	→	8	2	7	9	9201.87633	0.00180
11	0	11	11	→	10	0	10	10	10076.21368	-0.00103
11	1	11	11	→	10	1	10	10	10076.21368	-0.00080
11	0	11	10	→	10	0	10	9	10076.22156	0.00190
11	1	11	10	→	10	1	10	9	10076.22156	0.00213
11	0	11	12	→	10	0	10	11	10076.22875	-0.00134
11	1	11	12	→	10	1	10	11	10076.22875	-0.00112
10	2	9	10	→	9	2	8	9	10077.67197	0.00021
10	2	9	9	→	9	2	8	8	10077.69974	-0.00168
10	2	9	11	→	9	2	8	10	10077.70928	0.00025
10	1	9	10	→	9	1	8	9	10077.79182	0.00037
10	1	9	9	→	9	1	8	8	10077.81922	-0.00172
10	1	9	11	→	9	1	8	10	10077.82900	0.00044
9	3	7	9	→	8	3	6	8	10081.05180	-0.00002
9	3	7	8	→	8	3	6	7	10081.10203	-0.00079
9	3	7	10	→	8	3	6	9	10081.10861	0.00143
9	2	7	9	→	8	2	6	8	10097.57430	0.00009
9	2	7	8	→	8	2	6	7	10097.60164	-0.00101
9	2	7	10	→	8	2	6	9	10097.61077	0.00114
12	0	12	12	→	11	0	11	11	10952.37568	-0.00166
12	1	12	12	→	11	1	11	11	10952.37568	-0.00163
12	0	12	11	→	11	0	11	10	10952.38199	0.00035
12	1	12	11	→	11	1	11	10	10952.38199	0.00039
12	0	12	13	→	11	0	11	12	10952.39197	0.00147
12	1	12	13	→	11	1	11	12	10952.39197	0.00150
10	2	8	10	→	9	2	7	9	10963.47212	0.00143
10	2	8	9	→	9	2	7	8	10963.50527	-0.00124
10	2	8	11	→	9	2	7	10	10963.51197	0.00044
13	0	13	13	→	12	0	12	12	11828.54300	-0.00153
13	1	13	13	→	12	1	12	12	11828.54300	-0.00152
13	0	13	12	→	12	0	12	11	11828.54869	0.00041
13	1	13	12	→	12	1	12	11	11828.54869	0.00041
13	0	13	14	→	12	0	12	13	11828.55730	0.00139
13	1	13	14	→	12	1	12	13	11828.55730	0.00140
14	0	14	14	→	13	0	13	13	12704.71452	-0.00010
14	0	14	13	→	13	0	13	12	12704.71452	-0.00340
14	1	14	14	→	13	1	13	13	12704.71452	-0.00010
14	1	14	13	→	13	1	13	12	12704.71452	-0.00340
14	0	14	15	→	13	0	13	14	12704.72636	0.00181
14	1	14	15	→	13	1	13	14	12704.72636	0.00181
13	2	12	13	→	12	2	11	12	12705.45989	0.00121

13	1	12	13	→	12	1	11	12	12705.45989	0.00037
13	2	12	12	→	12	2	11	11	12705.47648	-0.00126
13	1	12	12	→	12	1	11	11	12705.47648	-0.00211
13	2	12	14	→	12	2	11	13	12705.48402	0.00101
13	1	12	14	→	12	1	11	13	12705.48402	0.00017
15	0	15	15	→	14	0	14	14	13580.88666	0.00007
15	0	15	14	→	14	0	14	13	13580.88666	-0.00286
15	1	15	15	→	14	1	14	14	13580.88666	0.00007
15	1	15	14	→	14	1	14	13	13580.88666	-0.00286
15	0	15	16	→	14	0	14	15	13580.89660	0.00126
15	1	15	16	→	14	1	14	15	13580.89660	0.00126

Table II(D). Microwave transitions of the $^{13}C_3$ isotopologue of PFBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
5	0	5	4	→	4	0	4	3	4820.25070	0.00029
5	0	5	5	→	4	0	4	4	4820.25070	-0.00020
5	0	5	6	→	4	0	4	5	4820.29893	-0.00031
7	1	7	7	→	6	1	6	6	6568.36199	-0.00207
7	1	7	6	→	6	1	6	5	6568.37508	0.00143
7	1	7	8	→	6	1	6	7	6568.39706	-0.00091
7	0	7	7	→	6	0	6	6	6568.58971	-0.00151
7	0	7	6	→	6	0	6	5	6568.60119	0.00096
7	0	7	8	→	6	0	6	7	6568.62431	-0.00033
6	1	5	5	→	5	1	4	4	6597.84744	-0.00045
6	1	5	6	→	5	1	4	5	6597.84744	0.00022
6	1	5	7	→	5	1	4	6	6597.87218	-0.00067
5	2	3	5	→	4	2	2	4	6688.62485	-0.00060
5	2	3	4	→	4	2	2	3	6688.64855	0.00068
5	2	3	6	→	4	2	2	5	6688.68295	-0.00017
6	3	4	6	→	5	3	3	5	7283.28945	-0.00007
6	3	4	7	→	5	3	3	6	7283.58695	0.00027
6	3	4	5	→	5	3	3	4	7283.62842	-0.00053
7	2	6	7	→	6	2	5	6	7443.08497	-0.00018
7	2	6	6	→	6	2	5	5	7443.14346	-0.00055
7	2	6	8	→	6	2	5	7	7443.15499	0.00010
8	1	8	8	→	7	1	7	7	7444.11336	-0.00017
8	1	8	7	→	7	1	7	6	7444.12226	0.00073
8	1	8	9	→	7	1	7	8	7444.14070	0.00020
8	0	8	8	→	7	0	7	7	7444.15808	0.00206
8	0	8	7	→	7	0	7	6	7444.16767	0.00374
8	0	8	9	→	7	0	7	8	7444.18208	-0.00083
6	2	4	5	→	5	2	3	4	7632.68835	0.00023
6	2	4	7	→	5	2	3	6	7632.73864	0.00010
6	2	4	6	→	5	2	3	5	7632.84410	0.00027
7	3	5	7	→	6	3	4	6	8266.91228	0.00005
7	3	5	8	→	6	3	4	7	8267.05595	-0.00047
7	3	5	6	→	6	3	4	5	8267.06571	0.00140
8	2	7	8	→	7	2	6	7	8321.46235	0.00009
8	2	7	7	→	7	2	6	6	8321.50463	-0.00108
8	2	7	9	→	7	2	6	8	8321.51617	0.00058
7	2	5	6	→	6	2	4	5	8434.54887	-0.00029
7	2	5	8	→	6	2	4	7	8434.57897	0.00011
7	2	5	7	→	6	2	4	6	8434.64321	0.00011
10	0	10	10	→	9	0	9	9	9195.54183	-0.00149
10	1	10	10	→	9	1	9	9	9195.54183	-0.00014
10	0	10	9	→	9	0	9	8	9195.55025	0.00115

10	1	10	9	→	9	1	9	8	9195.55025	0.00250
10	0	10	11	→	9	0	9	10	9195.55999	-0.00162
10	1	10	11	→	9	1	9	10	9195.55999	-0.00027
9	2	8	9	→	8	2	7	8	9197.32056	-0.00050
9	2	8	8	→	8	2	7	7	9197.35325	-0.00317
9	2	8	10	→	8	2	7	9	9197.36726	0.00212
11	0	11	11	→	10	0	10	10	10071.26706	-0.00108
11	1	11	11	→	10	1	10	10	10071.26706	-0.00085
11	0	11	10	→	10	0	10	9	10071.27493	0.00181
11	1	11	10	→	10	1	10	9	10071.27493	0.00205
11	0	11	12	→	10	0	10	11	10071.28220	-0.00138
11	1	11	12	→	10	1	10	11	10071.28220	-0.00114
10	2	9	10	→	9	2	8	9	10072.73311	0.00056
10	2	9	9	→	9	2	8	8	10072.76037	-0.00197
10	2	9	11	→	9	2	8	10	10072.77011	0.00015
10	1	9	10	→	9	1	8	9	10072.85538	0.00069
10	1	9	9	→	9	1	8	8	10072.88261	-0.00169
10	1	9	11	→	9	1	8	10	10072.89201	0.00007
9	3	7	9	→	8	3	6	8	10076.06824	0.00031
9	3	7	8	→	8	3	6	7	10076.11798	-0.00124
9	3	7	10	→	8	3	6	9	10076.12475	0.00118
12	0	12	12	→	11	0	11	11	10946.99920	-0.00130
12	1	12	12	→	11	1	11	11	10946.99920	-0.00126
12	0	12	11	→	11	0	11	10	10947.00473	-0.00008
12	1	12	11	→	11	1	11	10	10947.00473	-0.00004
12	0	12	13	→	11	0	11	12	10947.01517	0.00147
12	1	12	13	→	11	1	11	12	10947.01517	0.00151
10	2	8	10	→	9	2	7	9	10958.18357	0.00107
10	2	8	9	→	9	2	7	8	10958.21793	-0.00052
10	2	8	11	→	9	2	7	10	10958.22418	0.00070
13	0	13	13	→	12	0	12	12	11822.73619	-0.00125
13	1	13	13	→	12	1	12	12	11822.73619	-0.00124
13	0	13	12	→	12	0	12	11	11822.74146	0.00025
13	1	13	12	→	12	1	12	11	11822.74146	0.00025
13	0	13	14	→	12	0	12	13	11822.74956	0.00070
13	1	13	14	→	12	1	12	13	11822.74956	0.00071
14	0	14	14	→	13	0	13	13	12698.47764	0.00032
14	0	14	13	→	13	0	13	12	12698.47764	-0.00300
14	1	14	14	→	13	1	13	13	12698.47764	0.00032
14	1	14	13	→	13	1	13	12	12698.47764	-0.00300
14	0	14	15	→	13	0	13	14	12698.48860	0.00131
14	1	14	15	→	13	1	13	14	12698.48860	0.00131
13	2	12	13	→	12	2	11	12	12699.22653	0.00113
13	1	12	13	→	12	1	11	12	12699.22653	0.00026
13	2	12	12	→	12	2	11	11	12699.24363	-0.00091
13	1	12	12	→	12	1	11	11	12699.24363	-0.00178

13	2	12	14	→	12	2	11	13	12699.25129	0.00147
13	1	12	14	→	12	1	11	13	12699.25129	0.00061
15	0	15	15	→	14	0	14	14	13574.21942	0.00031
15	0	15	14	→	14	0	14	13	13574.21942	-0.00263
15	1	15	15	→	14	1	14	14	13574.21942	0.00031
15	1	15	14	→	14	1	14	13	13574.21942	-0.00263
15	0	15	16	→	14	0	14	15	13574.22917	0.00128
15	1	15	16	→	14	1	14	15	13574.22917	0.00128

Table II(E). Microwave transitions of the $^{13}C_4$ isotopologue of PFBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
5	0	5	4	→	4	0	4	3	4819.42279	0.00126
5	0	5	5	→	4	0	4	4	4819.42279	-0.00034
5	0	5	6	→	4	0	4	5	4819.46988	-0.00093
6	1	5	5	→	5	1	4	4	6598.10553	0.00272
6	1	5	6	→	5	1	4	5	6598.10553	0.00006
6	1	5	7	→	5	1	4	6	6598.12813	-0.00044
7	2	6	7	→	6	2	5	6	7441.17599	-0.00019
7	2	6	6	→	6	2	5	5	7441.23504	0.00013
7	2	6	8	→	6	2	5	7	7441.24572	-0.00025
8	1	8	8	→	7	1	7	7	7442.48949	-0.00075
8	1	8	7	→	7	1	7	6	7442.50200	0.00393
8	1	8	9	→	7	1	7	8	7442.51765	0.00052
8	0	8	8	→	7	0	7	7	7442.53703	-0.00126
8	0	8	7	→	7	0	7	6	7442.54605	0.00003
8	0	8	9	→	7	0	7	8	7442.56440	-0.00069
6	2	4	5	→	5	2	3	4	7633.75335	0.00016
6	2	4	7	→	5	2	3	6	7633.80348	0.00013
6	2	4	6	→	5	2	3	5	7633.90459	-0.00007
7	3	5	7	→	6	3	4	6	8261.37659	-0.00015
7	3	5	8	→	6	3	4	7	8261.52281	-0.00044
7	3	5	6	→	6	3	4	5	8261.53239	0.00103
7	2	5	6	→	6	2	4	5	8437.99538	0.00004
7	2	5	8	→	6	2	4	7	8438.02579	-0.00006
7	2	5	7	→	6	2	4	6	8438.09288	-0.00015
10	0	10	10	→	9	0	9	9	9193.53347	-0.00161
10	1	10	10	→	9	1	9	9	9193.53347	-0.00003
10	0	10	9	→	9	0	9	8	9193.54122	0.00046
10	1	10	9	→	9	1	9	8	9193.54122	0.00204
10	0	10	11	→	9	0	9	10	9193.55212	-0.00120
10	1	10	11	→	9	1	9	10	9193.55212	0.00038
9	2	8	9	→	8	2	7	8	9195.36167	0.00039
9	2	8	8	→	8	2	7	7	9195.39433	-0.00195
9	2	8	10	→	8	2	7	9	9195.40597	0.00085
11	0	11	11	→	10	0	10	10	10069.06581	-0.00098
11	1	11	11	→	10	1	10	10	10069.06581	-0.00070
11	0	11	10	→	10	0	10	9	10069.07337	0.00169
11	1	11	10	→	10	1	10	9	10069.07337	0.00197
11	0	11	12	→	10	0	10	11	10069.08097	-0.00122
11	1	11	12	→	10	1	10	11	10069.08097	-0.00094
10	2	9	10	→	9	2	8	9	10070.58546	0.00051
10	2	9	9	→	9	2	8	8	10070.61219	-0.00225
10	2	9	11	→	9	2	8	10	10070.62222	0.00007

10	1	9	10	→	9	1	8	9	10070.72563	0.00028
10	1	9	9	→	9	1	8	8	10070.75321	-0.00143
10	1	9	11	→	9	1	8	10	10070.76272	0.00035
9	3	7	9	→	8	3	6	8	10073.59807	0.00002
9	3	7	8	→	8	3	6	7	10073.64765	-0.00158
9	3	7	10	→	8	3	6	9	10073.65477	0.00108
12	0	12	12	→	11	0	11	11	10944.60508	-0.00132
12	1	12	12	→	11	1	11	11	10944.60508	-0.00127
12	0	12	11	→	11	0	11	10	10944.61113	0.00048
12	1	12	11	→	11	1	11	10	10944.61113	0.00053
12	0	12	13	→	11	0	11	12	10944.62124	0.00167
12	1	12	13	→	11	1	11	12	10944.62124	0.00172
10	2	8	10	→	9	2	7	9	10956.44586	0.00071
10	2	8	9	→	9	2	7	8	10956.47908	-0.00107
10	2	8	11	→	9	2	7	10	10956.48622	0.00087
13	0	13	13	→	12	0	12	12	11820.14951	-0.00128
13	1	13	13	→	12	1	12	12	11820.14951	-0.00127
13	0	13	12	→	12	0	12	11	11820.15412	-0.00038
13	1	13	12	→	12	1	12	11	11820.15412	-0.00037
13	0	13	14	→	12	0	12	13	11820.16315	0.00097
13	1	13	14	→	12	1	12	13	11820.16315	0.00098
14	0	14	14	→	13	0	13	13	12695.69771	-0.00051
14	0	14	13	→	13	0	13	12	12695.69771	-0.00378
14	1	14	14	→	13	1	13	13	12695.69771	-0.00051
14	1	14	13	→	13	1	13	12	12695.69771	-0.00378
14	0	14	15	→	13	0	13	14	12695.70942	0.00125
14	1	14	15	→	13	1	13	14	12695.70942	0.00125
13	2	12	13	→	12	2	11	12	12696.47815	0.00139
13	1	12	13	→	12	1	11	12	12696.47815	0.00033
13	2	12	12	→	12	2	11	11	12696.49520	-0.00054
13	1	12	12	→	12	1	11	11	12696.49520	-0.00159
13	2	12	14	→	12	2	11	13	12696.50314	0.00208
13	1	12	14	→	12	1	11	13	12696.50314	0.00103
15	0	15	15	→	14	0	14	14	13571.24798	0.00035
15	0	15	14	→	14	0	14	13	13571.24798	-0.00255
15	1	15	15	→	14	1	14	14	13571.24798	0.00035
15	1	15	14	→	14	1	14	13	13571.24798	-0.00255
15	0	15	16	→	14	0	14	15	13571.25804	0.00165
15	1	15	16	→	14	1	14	15	13571.25804	0.00165

Table II(F). Microwave transitions of the $^{13}C_5$ isotopologue of PFBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
5	0	5	4	→	4	0	4	3	4801.08732	0.00278
5	0	5	5	→	4	0	4	4	4801.08732	-0.00019
5	0	5	6	→	4	0	4	5	4801.13484	0.00037
7	1	7	7	→	6	1	6	6	6541.55260	-0.00128
7	1	7	6	→	6	1	6	5	6541.56375	0.00076
7	1	7	8	→	6	1	6	7	6541.58715	-0.00050
7	0	7	7	→	6	0	6	6	6541.83626	-0.00181
7	0	7	6	→	6	0	6	5	6541.84723	0.00074
7	0	7	8	→	6	0	6	7	6541.87086	-0.00040
7	2	6	7	→	6	2	5	6	7412.05938	-0.00001
7	2	6	6	→	6	2	5	5	7412.11764	-0.00049
7	2	6	8	→	6	2	5	7	7412.12941	-0.00002
8	1	8	8	→	7	1	7	7	7413.74130	-0.00043
8	1	8	7	→	7	1	7	6	7413.75080	0.00144
8	1	8	9	→	7	1	7	8	7413.76853	-0.00005
8	0	8	8	→	7	0	7	7	7413.79607	-0.00100
8	0	8	7	→	7	0	7	6	7413.80578	0.00119
8	0	8	9	→	7	0	7	8	7413.82295	-0.00087
6	2	4	5	→	5	2	3	4	7607.13293	-0.00130
6	2	4	7	→	5	2	3	6	7607.18528	0.00116
6	2	4	6	→	5	2	3	5	7607.27973	-0.00080
7	3	5	7	→	6	3	4	6	8224.81810	0.00061
7	3	5	8	→	6	3	4	7	8224.96624	-0.00089
7	3	5	6	→	6	3	4	5	8224.97649	0.00096
7	2	5	6	→	6	2	4	5	8411.77221	0.00065
7	2	5	8	→	6	2	4	7	8411.80284	-0.00023
7	2	5	7	→	6	2	4	6	8411.87374	0.00012
10	0	10	10	→	9	0	9	9	9158.01828	-0.00132
10	1	10	10	→	9	1	9	9	9158.01828	0.00059
10	0	10	9	→	9	0	9	8	9158.02662	0.00146
10	1	10	9	→	9	1	9	8	9158.02662	0.00336
10	0	10	11	→	9	0	9	10	9158.03659	-0.00123
10	1	10	11	→	9	1	9	10	9158.03659	0.00068
9	2	8	9	→	8	2	7	8	9159.89637	-0.00001
9	2	8	8	→	8	2	7	7	9159.92985	-0.00118
9	2	8	10	→	8	2	7	9	9159.94104	0.00102
11	0	11	11	→	10	0	10	10	10030.16527	-0.00163
11	1	11	11	→	10	1	10	10	10030.16527	-0.00129
11	0	11	10	→	10	0	10	9	10030.17197	0.00027
11	1	11	10	→	10	1	10	9	10030.17197	0.00061
11	0	11	12	→	10	0	10	11	10030.18328	0.00099
11	1	11	12	→	10	1	10	11	10030.18328	0.00134

10	2	9	10	→	9	2	8	9	10031.74644	0.00056
10	2	9	9	→	9	2	8	8	10031.77264	-0.00244
10	2	9	11	→	9	2	8	10	10031.78334	0.00043
10	1	9	10	→	9	1	8	9	10031.91122	0.00051
10	1	9	9	→	9	1	8	8	10031.93739	-0.00229
10	1	9	11	→	9	1	8	10	10031.94789	0.00035
9	2	7	9	→	8	2	6	8	10054.92512	0.00167
9	2	7	8	→	8	2	6	7	10054.94628	-0.00154
9	2	7	10	→	8	2	6	9	10054.95590	0.00036
12	0	12	12	→	11	0	11	11	10902.32193	-0.00067
12	1	12	12	→	11	1	11	11	10902.32193	-0.00061
12	0	12	11	→	11	0	11	10	10902.32679	0.00002
12	1	12	11	→	11	1	11	10	10902.32679	0.00008
12	0	12	13	→	11	0	11	12	10902.33622	0.00046
12	1	12	13	→	11	1	11	12	10902.33622	0.00052
10	2	8	10	→	9	2	7	9	10914.95904	0.00045
10	2	8	9	→	9	2	7	8	10914.99188	-0.00061
10	2	8	11	→	9	2	7	10	10914.99912	0.00121
13	0	13	13	→	12	0	12	12	11774.48276	-0.00061
13	0	13	12	→	12	0	12	11	11774.48276	-0.00426
13	1	13	13	→	12	1	12	12	11774.48276	-0.00059
13	1	13	12	→	12	1	12	11	11774.48276	-0.00425
13	0	13	14	→	12	0	12	13	11774.49634	0.00159
13	1	13	14	→	12	1	12	13	11774.49634	0.00160
14	0	14	14	→	13	0	13	13	12646.64593	-0.00145
14	0	14	13	→	13	0	13	12	12646.64593	-0.00467
14	1	14	14	→	13	1	13	13	12646.64593	-0.00145
14	1	14	13	→	13	1	13	12	12646.64593	-0.00467
14	0	14	15	→	13	0	13	14	12646.66007	0.00275
14	1	14	15	→	13	1	13	14	12646.66007	0.00275
15	0	15	15	→	14	0	14	14	13518.81359	0.00006
15	0	15	14	→	14	0	14	13	13518.81359	-0.00279
15	1	15	15	→	14	1	14	14	13518.81359	0.00006
15	1	15	14	→	14	1	14	13	13518.81359	-0.00279
15	0	15	16	→	14	0	14	15	13518.82421	0.00193
15	1	15	16	→	14	1	14	15	13518.82421	0.00193

Table II(G). Microwave transitions of the ^{15}N isotopologue of PFBN in MHz

J'	$K_{a'}$	$K_{c'}$	→	J"	$K_{a"}$	$K_{c"}$	$\nu_{obs.}$	$\nu_{obs.-calc.}$
7	2	6	→	6	2	5	7364.76191	0.00380
8	1	8	→	7	1	7	7367.08546	0.00041
8	0	8	→	7	0	7	7367.15458	0.00032
7	1	6	→	6	1	5	7380.53567	0.00009
9	1	9	→	8	1	8	8233.72603	-0.00120
9	0	9	→	8	0	8	8233.74167	0.00095
8	2	7	→	7	2	6	8235.24969	0.00322
8	1	7	→	7	1	6	8239.28610	0.00192
10	0	10	→	9	0	9	9100.37433	0.00078
10	1	10	→	9	1	9	9100.37433	0.00334
9	2	8	→	8	2	7	9102.34863	0.00315
9	1	8	→	8	1	7	9103.30106	0.00250
11	0	11	→	10	0	10	9967.02542	0.00060
11	1	11	→	10	1	10	9967.02542	0.00107
10	2	9	→	9	2	8	9968.72322	0.00293
10	1	9	→	9	1	8	9968.93534	0.00251
12	1	12	→	11	1	11	10833.68674	0.00122
12	0	12	→	11	0	11	10833.68674	0.00113
11	2	10	→	10	2	9	10835.04765	0.00273
11	1	10	→	10	1	9	10835.09371	0.00336
13	0	13	→	12	0	12	11700.35264	0.00053
13	1	13	→	12	1	12	11700.35264	0.00054
12	2	11	→	11	2	10	11701.44423	0.00303
12	1	11	→	11	1	10	11701.45551	0.00491
14	0	14	→	13	0	13	12567.02333	0.00102
14	1	14	→	13	1	13	12567.02333	0.00103
13	2	12	→	12	2	11	12567.91226	0.00380
13	1	12	→	12	1	11	12567.91226	0.00191
15	0	15	→	14	0	14	13433.69613	0.00119
15	1	15	→	14	1	14	13433.69613	0.00119

Appendix III. Microwave transitions of the 2-fluorobenzonitrile (2FBN) and its isotopologues

Table III(A). Microwave transitions of the parent 2FBN in MHz

J'	K_a'	K_c'	F'	→	J"	K_a"	K_c"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
2	0	2	2	→	1	0	1	2	4905.86534	-0.00053
2	0	2	1	→	1	0	1	0	4905.98867	0.00087
2	0	2	2	→	1	0	1	1	4907.12284	0.00245
2	0	2	3	→	1	0	1	2	4907.15418	0.00022
2	0	2	1	→	1	0	1	1	4909.12529	0.00070
2	1	1	2	→	1	1	0	1	5535.70300	0.00038
2	1	1	3	→	1	1	0	2	5537.00533	0.00104
2	1	1	1	→	1	1	0	0	5538.28810	0.00202
3	0	3	3	→	2	1	2	2	6075.45601	-0.00009
3	0	3	4	→	2	1	2	3	6076.09376	0.00028
3	0	3	2	→	2	1	2	1	6076.18579	-0.00086
3	1	3	3	→	2	1	2	3	6696.42411	-0.00056
3	1	3	3	→	2	1	2	2	6697.05762	0.00006
3	1	3	2	→	2	1	2	1	6697.40678	-0.00180
3	1	3	4	→	2	1	2	3	6697.41517	0.00092
3	1	3	2	→	2	1	2	2	6698.39328	-0.00071
3	0	3	3	→	2	0	2	3	7104.31487	-0.00063
3	0	3	2	→	2	0	2	1	7105.31542	0.00005
3	0	3	4	→	2	0	2	3	7105.58636	0.00058
3	0	3	3	→	2	0	2	2	7105.60303	-0.00056
3	0	3	2	→	2	0	2	2	7107.31906	-0.00051
7	2	5	7	→	7	2	6	7	7254.83259	0.00030
7	2	5	8	→	7	2	6	8	7254.97781	0.00123
7	2	5	6	→	7	2	6	6	7254.99484	-0.00254
3	2	2	3	→	2	2	1	2	7532.99562	0.00036
3	2	2	4	→	2	2	1	3	7534.33989	0.00088
3	2	2	2	→	2	2	1	1	7535.08634	0.00039
3	1	3	2	→	2	0	2	1	7726.53763	0.00034
3	1	3	4	→	2	0	2	3	7726.90673	0.00019
3	1	3	3	→	2	0	2	2	7727.20511	0.00005
4	2	3	3	→	4	1	4	3	7789.31030	-0.00024
4	2	3	5	→	4	1	4	5	7789.45829	-0.00155
4	2	3	4	→	4	1	4	4	7790.04021	-0.00031
3	2	1	3	→	2	2	0	2	7961.44373	0.00013
3	2	1	4	→	2	2	0	3	7962.85588	0.00076
3	2	1	2	→	2	2	0	1	7963.61407	-0.00018
4	2	3	3	→	4	0	4	3	8110.26973	0.00008

4	2	3	5	→	4	0	4	5	8110.44911	-0.00011
4	2	3	4	→	4	0	4	4	8111.14688	-0.00048
3	1	2	3	→	2	1	1	3	8221.73116	-0.00121
3	1	2	3	→	2	1	1	2	8222.44406	0.00051
3	1	2	2	→	2	1	1	1	8222.77286	0.00149
3	1	2	4	→	2	1	1	3	8222.79502	0.00017
3	1	2	2	→	2	1	1	2	8223.87746	-0.00077
4	0	4	4	→	3	1	3	3	8506.55045	0.00031
4	0	4	3	→	3	1	3	2	8506.79155	0.00097
4	0	4	5	→	3	1	3	4	8506.81455	-0.00002
4	3	2	3	→	4	2	3	3	8771.10089	0.00023
4	3	2	5	→	4	2	3	5	8771.36333	0.00006
4	3	2	4	→	4	2	3	4	8772.38488	0.00049
4	1	4	4	→	3	1	3	4	8826.66620	-0.00120
4	1	4	4	→	3	1	3	3	8827.65692	-0.00006
4	1	4	3	→	3	1	3	2	8827.74925	-0.00044
4	1	4	5	→	3	1	3	4	8827.80433	0.00038
4	1	4	3	→	3	1	3	3	8829.08543	-0.00070
4	0	4	4	→	3	0	3	4	9126.87957	-0.00175
4	0	4	3	→	3	0	3	2	9128.01240	-0.00010
4	0	4	5	→	3	0	3	4	9128.13572	0.00039
4	0	4	4	→	3	0	3	3	9128.15141	-0.00019
4	0	4	3	→	3	0	3	3	9129.72697	-0.00151
5	2	4	4	→	5	1	5	4	9183.83911	0.00072
5	2	4	6	→	5	1	5	6	9183.91482	-0.00052
5	2	4	5	→	5	1	5	5	9184.29320	0.00009
5	2	4	4	→	5	0	5	4	9332.13773	-0.00031
5	2	4	6	→	5	0	5	6	9332.22403	-0.00034
5	2	4	5	→	5	0	5	5	9332.64752	-0.00049
4	1	4	3	→	3	0	3	2	9448.97132	-0.00030
4	1	4	5	→	3	0	3	4	9449.12497	0.00026
4	1	4	4	→	3	0	3	3	9449.25825	-0.00019
6	1	5	5	→	6	1	6	5	9647.39347	-0.00301
6	1	5	7	→	6	1	6	7	9647.40628	0.00127
6	1	5	6	→	6	1	6	6	9647.45640	0.00088
2	2	1	3	→	1	1	0	2	9820.71753	0.00080
2	2	1	1	→	1	1	0	0	9820.85904	0.00267
2	2	1	2	→	1	1	0	1	9821.47104	0.00100
8	2	6	8	→	8	2	7	8	9848.20562	0.00059
8	2	6	9	→	8	2	7	9	9848.29744	-0.00160
8	2	6	7	→	8	2	7	7	9848.31427	0.00341
4	2	3	4	→	3	2	2	3	9953.91287	-0.00037
4	2	3	5	→	3	2	2	4	9954.46977	0.00061

4	2	3	3	→	3	2	2	2	9954.61141	-0.00058
4	3	2	4	→	3	3	1	3	10233.96318	0.00022
4	3	2	5	→	3	3	1	4	10235.22606	0.00107
4	3	2	3	→	3	3	1	2	10235.70957	-0.00058
4	3	1	4	→	3	3	0	3	10330.93092	0.00009
4	3	1	5	→	3	3	0	4	10332.21870	0.00092
4	3	1	3	→	3	3	0	2	10332.70824	-0.00031
5	1	4	5	→	4	2	3	4	10399.85695	0.00056
5	1	4	6	→	4	2	3	5	10400.51728	0.00142
5	1	4	4	→	4	2	3	3	10400.62002	-0.00039
2	2	0	3	→	1	1	1	2	10450.41614	0.00132
2	2	0	1	→	1	1	1	0	10450.69694	0.00212
2	2	0	2	→	1	1	1	1	10451.04108	0.00181
5	0	5	5	→	4	1	4	4	10758.11227	-0.00009
5	0	5	4	→	4	1	4	3	10758.19463	-0.00070
5	0	5	6	→	4	1	4	5	10758.23241	0.00063
4	1	3	4	→	3	1	2	4	10785.80684	-0.00145
4	1	3	4	→	3	1	2	3	10786.87089	0.00013
4	1	3	3	→	3	1	2	2	10786.92779	0.00015
4	1	3	5	→	3	1	2	4	10786.99510	0.00051
4	1	3	3	→	3	1	2	3	10788.36145	-0.00088
6	2	5	5	→	6	0	6	5	10864.90153	-0.00191
6	2	5	7	→	6	0	6	7	10864.95180	0.00002
6	2	5	6	→	6	0	6	6	10865.23677	-0.00115
4	2	2	4	→	3	2	1	4	10869.03183	-0.00065
4	2	2	4	→	3	2	1	3	10869.15633	0.00043
4	2	2	5	→	3	2	1	4	10869.75988	0.00077
4	2	2	3	→	3	2	1	2	10869.90308	0.00045
4	2	2	3	→	3	2	1	3	10870.06938	-0.00028
5	1	5	5	→	4	1	4	5	10905.32989	-0.00083
5	1	5	5	→	4	1	4	4	10906.46778	0.00052
5	1	5	4	→	4	1	4	3	10906.49353	-0.00144
5	1	5	6	→	4	1	4	5	10906.54126	0.00045
5	1	5	4	→	4	1	4	4	10907.92172	-0.00240
5	0	5	5	→	4	0	4	5	11077.96357	-0.00162
5	0	5	4	→	4	0	4	3	11079.15447	0.00002
5	0	5	6	→	4	0	4	5	11079.22043	-0.00073
5	0	5	5	→	4	0	4	4	11079.22043	0.00123
5	0	5	4	→	4	0	4	4	11080.72943	-0.00189
5	3	3	4	→	5	1	4	4	11181.79892	-0.00076
5	3	3	6	→	5	1	4	6	11182.00940	-0.00050
5	3	3	5	→	5	1	4	5	11183.04106	-0.00082
6	3	4	5	→	6	1	5	5	11221.09636	-0.00093

6	3	4	7	→	6	1	5	7	11221.20555	-0.00103
6	3	4	6	→	6	1	5	6	11221.85333	-0.00057
5	1	5	4	→	4	0	4	3	11227.45370	-0.00039
5	1	5	6	→	4	0	4	5	11227.53142	0.00124
5	1	5	5	→	4	0	4	4	11227.57316	-0.00094
7	3	5	6	→	7	1	6	6	11768.52030	-0.00087
7	3	5	8	→	7	1	6	8	11768.57914	-0.00019
7	3	5	7	→	7	1	6	7	11768.98165	-0.00079
3	2	2	2	→	2	1	1	1	11817.65696	0.00072
3	2	2	4	→	2	1	1	3	11818.05209	0.00063
3	2	2	3	→	2	1	1	2	11818.76222	-0.00046
7	1	6	6	→	7	1	7	6	11960.80354	-0.00307
7	1	6	8	→	7	1	7	8	11960.82218	0.00154
7	1	6	7	→	7	1	7	7	11960.91820	0.00032
5	2	4	5	→	4	2	3	5	12300.16263	-0.00136
5	2	4	5	→	4	2	3	4	12300.72018	0.00032
5	2	4	6	→	4	2	3	5	12300.99691	0.00061
5	2	4	4	→	4	2	3	3	12301.02204	-0.00079
5	2	4	4	→	4	2	3	4	12301.72124	-0.00076
7	2	6	6	→	7	0	7	6	12609.52606	0.00140
7	2	6	8	→	7	0	7	8	12609.55476	-0.00100
7	2	6	7	→	7	0	7	7	12609.76957	-0.00156
8	3	6	7	→	8	1	7	7	12808.39598	0.00170
8	3	6	9	→	8	1	7	9	12808.42527	-0.00130
8	3	6	8	→	8	1	7	8	12808.68250	-0.00031
5	3	3	5	→	4	3	2	4	12810.51412	0.00024
5	3	3	6	→	4	3	2	5	12811.16288	0.00038
5	3	3	4	→	4	3	2	3	12811.31890	-0.00053
5	4	2	5	→	4	4	1	4	12811.61583	0.00123
5	4	2	6	→	4	4	1	5	12812.76528	0.00141
5	4	2	4	→	4	4	1	3	12813.10485	0.00083
5	4	1	5	→	4	4	0	4	12827.28989	-0.00034
5	4	1	6	→	4	4	0	5	12828.44381	-0.00008
5	4	1	4	→	4	4	0	3	12828.78443	-0.00046
6	0	6	6	→	5	1	5	5	12884.18750	-0.00063
6	0	6	5	→	5	1	5	4	12884.21591	0.00026
6	0	6	7	→	5	1	5	6	12884.24783	0.00003
6	1	6	6	→	5	1	5	6	12946.67643	-0.00128
6	1	6	6	→	5	1	5	5	12947.88522	-0.00258
6	1	6	5	→	5	1	5	4	12947.89673	0.00133
6	1	6	5	→	5	1	5	5	12949.35128	-0.00098
6	0	6	6	→	5	0	5	6	13031.28598	-0.00109
6	0	6	5	→	5	0	5	4	13032.51593	0.00063

6	0	6	6	→	5	0	5	5	13032.54204	-0.00100
6	0	6	7	→	5	0	5	6	13032.55708	0.00026
6	0	6	5	→	5	0	5	5	13034.02594	-0.00148
6	1	6	5	→	5	0	5	4	13096.19492	-0.00012
6	1	6	7	→	5	0	5	6	13096.24138	0.00191
6	1	6	6	→	5	0	5	5	13096.24138	-0.00132
5	3	2	5	→	4	3	1	4	13123.76954	0.00035
5	3	2	6	→	4	3	1	5	13124.46401	0.00057
5	3	2	4	→	4	3	1	3	13124.62823	0.00033
5	1	4	5	→	4	1	3	5	13162.03043	-0.00126
5	1	4	4	→	4	1	3	3	13163.18879	-0.00084
5	1	4	5	→	4	1	3	4	13163.21836	0.00036
5	1	4	6	→	4	1	3	5	13163.24738	0.00034
5	1	4	4	→	4	1	3	4	13164.68006	-0.00113
6	1	5	6	→	5	2	4	5	13411.05014	-0.00007
6	1	5	7	→	5	2	4	6	13411.42122	0.00111
6	1	5	5	→	5	2	4	4	13411.45196	-0.00152
4	2	3	3	→	3	1	2	2	13549.49635	-0.00050
4	2	3	5	→	3	1	2	4	13549.72660	0.00083
4	2	3	4	→	3	1	2	3	13550.23304	0.00067
5	2	3	5	→	4	2	2	5	13761.83780	-0.00135
5	2	3	5	→	4	2	2	4	13762.56517	-0.00061
5	2	3	6	→	4	2	2	5	13762.85758	-0.00028
5	2	3	4	→	4	2	2	3	13762.87869	0.00024
5	2	3	4	→	4	2	2	4	13763.79046	-0.00175
3	2	1	2	→	2	1	2	1	13904.05689	0.00175
3	2	1	4	→	2	1	2	3	13904.36367	-0.00037
3	2	1	3	→	2	1	2	2	13904.87302	-0.00051
8	1	7	7	→	8	1	8	7	14167.56427	0.00103
8	1	7	9	→	8	1	8	9	14167.58041	0.00159
8	1	7	8	→	8	1	8	8	14167.70124	-0.00126
6	2	5	6	→	5	2	4	6	14564.29897	-0.00165
6	2	5	6	→	5	2	4	5	14565.13316	0.00022
6	2	5	5	→	5	2	4	4	14565.28074	0.00004
6	2	5	7	→	5	2	4	6	14565.28542	0.00119
6	2	5	5	→	5	2	4	5	14566.28127	-0.00157
7	0	7	7	→	6	1	6	6	14940.53475	-0.00038
7	0	7	6	→	6	1	6	5	14940.54617	0.00265
7	0	7	8	→	6	1	6	7	14940.56907	-0.00034
7	1	7	6	→	6	1	6	5	14966.57981	-0.00095
7	1	7	7	→	6	1	6	6	14966.57981	0.00043
7	1	7	8	→	6	1	6	7	14966.60779	0.00025
7	0	7	6	→	6	0	6	5	15004.22203	-0.00124

7	0	7	7	→	6	0	6	6	15004.23495	0.00015
7	0	7	8	→	6	0	6	7	15004.25261	0.00056
7	1	7	6	→	6	0	6	5	15030.25956	-0.00095
7	1	7	7	→	6	0	6	6	15030.27808	-0.00097
7	1	7	8	→	6	0	6	7	15030.29104	0.00085
5	2	4	4	→	4	1	3	3	15063.59146	-0.00058
5	2	4	6	→	4	1	3	5	15063.72783	0.00035
5	2	4	5	→	4	1	3	4	15064.08221	0.00074
6	1	5	5	→	5	1	4	4	15311.85709	0.00119
6	1	5	7	→	5	1	4	6	15311.89969	-0.00086
6	1	5	6	→	5	1	4	5	15311.91412	0.00044
6	3	4	6	→	5	3	3	5	15350.72737	0.00167
6	3	4	7	→	5	3	3	6	15351.09872	0.00149
6	3	4	5	→	5	3	3	4	15351.15441	0.00090
6	5	2	6	→	5	5	1	5	15362.23200	-0.00010
6	5	2	7	→	5	5	1	6	15363.27474	0.00154
6	5	2	5	→	5	5	1	4	15363.52379	-0.00060
6	5	1	6	→	5	5	0	5	15364.35909	-0.00052
6	5	1	7	→	5	5	0	6	15365.40171	0.00041
6	5	1	5	→	5	5	0	4	15365.65239	-0.00019
6	4	3	6	→	5	4	2	5	15440.18142	0.00006
6	4	3	7	→	5	4	2	6	15440.85713	0.00081
6	4	3	5	→	5	4	2	4	15440.99876	-0.00057
6	4	2	6	→	5	4	1	5	15507.79116	-0.00001
6	4	2	7	→	5	4	1	6	15508.47915	0.00039
6	4	2	5	→	5	4	1	4	15508.62311	-0.00056
3	3	1	4	→	2	2	0	3	15909.30822	0.00083
3	3	1	2	→	2	2	0	1	15909.41855	0.00012
3	3	1	3	→	2	2	0	2	15909.74803	0.00147
3	3	0	4	→	2	2	1	3	16041.70658	-0.00041
3	3	0	2	→	2	2	1	1	16041.85302	0.00114
3	3	0	3	→	2	2	1	2	16042.08334	0.00112
6	3	3	6	→	5	3	2	5	16068.83235	-0.00026
6	3	3	7	→	5	3	2	6	16069.26068	0.00040
6	3	3	5	→	5	3	2	4	16069.32084	-0.00244
6	2	5	5	→	5	1	4	4	16465.68358	0.00047
6	2	5	7	→	5	1	4	6	16465.76408	-0.00059
6	2	5	6	→	5	1	4	5	16465.99614	-0.00027
6	2	4	6	→	5	2	3	5	16533.03655	0.00009
6	2	4	5	→	5	2	3	4	16533.16443	-0.00121
6	2	4	7	→	5	2	3	6	16533.17852	0.00109
7	2	6	7	→	6	2	5	6	16748.76793	-0.00008
7	2	6	6	→	6	2	5	5	16748.84327	-0.00122

7	2	6	8	→	6	2	5	7	16748.85696	0.00093
8	1	8	7	→	7	1	7	6	16973.27093	-0.00023
8	1	8	8	→	7	1	7	7	16973.27093	-0.00047
8	1	8	9	→	7	1	7	8	16973.29249	0.00046
8	0	8	7	→	7	0	7	6	16989.02348	-0.00140
8	0	8	8	→	7	0	7	7	16989.03093	0.00122
8	0	8	9	→	7	0	7	8	16989.04594	-0.00043
8	1	8	7	→	7	0	7	6	16999.30633	-0.00207
8	1	8	8	→	7	0	7	7	16999.31664	0.00098
8	1	8	9	→	7	0	7	8	16999.33107	0.00090
7	1	6	6	→	6	1	5	5	17279.99155	0.00065
7	1	6	8	→	6	1	5	7	17280.02369	0.00052
7	1	6	7	→	6	1	5	6	17280.04185	0.00011
7	3	5	7	→	6	3	4	6	17827.17044	0.00016
7	3	5	8	→	6	3	4	7	17827.39648	0.00056
7	3	5	6	→	6	3	4	5	17827.41450	-0.00028
7	2	6	6	→	6	1	5	5	17902.67167	-0.00004
7	2	6	8	→	6	1	5	7	17902.71926	-0.00089
7	2	6	7	→	6	1	5	6	17902.85197	0.00124
7	5	3	7	→	6	5	2	6	17994.92253	0.00058
7	5	3	8	→	6	5	2	7	17995.58802	0.00038
7	5	3	6	→	6	5	2	5	17995.71133	0.00017
7	5	2	7	→	6	5	1	6	18006.29127	-0.00046
7	5	2	8	→	6	5	1	7	18006.95956	-0.00012
7	5	2	6	→	6	5	1	5	18007.08338	-0.00014
7	4	4	7	→	6	4	3	6	18078.21441	0.00021
7	4	4	8	→	6	4	3	7	18078.64374	0.00055
7	4	4	6	→	6	4	3	5	18078.70966	0.00076
4	3	2	3	→	3	2	1	2	18181.51497	0.00064
4	3	2	5	→	3	2	1	4	18181.67736	0.00010
4	3	2	4	→	3	2	1	3	18182.26672	0.00080
7	4	3	7	→	6	4	2	6	18287.32100	-0.00042
7	4	3	8	→	6	4	2	7	18287.77708	-0.00009
7	4	3	6	→	6	4	2	5	18287.84549	-0.00080
8	2	7	8	→	7	2	6	7	18863.42039	-0.00004
8	2	7	7	→	7	2	6	6	18863.46095	-0.00106
8	2	7	9	→	7	2	6	8	18863.47492	0.00012
9	1	9	8	→	8	1	8	7	18974.30052	0.00006
9	1	9	9	→	8	1	8	8	18974.30052	-0.00038
9	1	9	10	→	8	1	8	9	18974.31636	-0.00074
9	0	9	8	→	8	0	8	7	18980.62654	0.00046
9	0	9	9	→	8	0	8	8	18980.62654	-0.00157
9	0	9	10	→	8	0	8	9	18980.64283	-0.00008

7	3	4	7	→	6	3	3	6	19100.63053	-0.00009
7	3	4	8	→	6	3	3	7	19100.90284	0.00141
7	3	4	6	→	6	3	3	5	19100.92109	-0.00239
7	2	5	7	→	6	2	4	6	19114.57701	0.00051
7	2	5	6	→	6	2	4	5	19114.61276	0.00041
7	2	5	8	→	6	2	4	7	19114.63290	0.00017
8	1	7	7	→	7	1	6	6	19180.02922	0.00143
8	1	7	9	→	7	1	6	8	19180.04894	-0.00127
8	1	7	8	→	7	1	6	7	19180.05638	0.00035
8	3	6	8	→	7	3	5	7	20219.75674	0.00034
8	3	6	9	→	7	3	5	8	20219.89891	0.00146
8	3	6	7	→	7	3	5	6	20219.89891	-0.00199
8	6	3	8	→	7	6	2	7	20536.51025	-0.00057
8	6	3	9	→	7	6	2	8	20537.15427	0.00088
8	6	3	7	→	7	6	2	6	20537.25936	0.00046
8	6	2	8	→	7	6	1	7	20538.16026	0.00040
8	6	2	9	→	7	6	1	8	20538.80173	-0.00103
8	6	2	7	→	7	6	1	6	20538.90781	-0.00050
8	5	4	8	→	7	5	3	7	20654.14172	0.00027
8	5	4	9	→	7	5	3	8	20654.59492	0.00060
8	5	4	7	→	7	5	3	6	20654.65917	-0.00048
8	5	3	8	→	7	5	2	7	20697.59510	0.00019
8	5	3	9	→	7	5	2	8	20698.05466	0.00043
8	5	3	7	→	7	5	2	6	20698.12039	0.00011
8	4	5	8	→	7	4	4	7	20702.14348	0.00038
8	4	5	9	→	7	4	4	8	20702.42974	0.00088
8	4	5	7	→	7	4	4	6	20702.45777	-0.00208
9	2	8	9	→	8	2	7	8	20927.03302	-0.00004
9	2	8	10	→	8	2	7	9	20927.07055	0.00124
10	1	10	9	→	9	1	9	8	20972.88932	-0.00097
10	1	10	10	→	9	1	9	9	20972.88932	-0.00123
10	1	10	11	→	9	1	9	10	20972.90555	0.00171
10	0	10	9	→	9	0	9	8	20975.35439	-0.00077
10	0	10	10	→	9	0	9	9	20975.35439	-0.00156
10	0	10	11	→	9	0	9	10	20975.37050	0.00174
9	1	8	9	→	8	1	7	8	21092.48816	-0.00071
9	1	8	10	→	8	1	7	9	21092.49772	0.00218
8	4	4	8	→	7	4	3	7	21208.82633	0.00020
8	4	4	9	→	7	4	3	8	21209.15679	0.00189
8	4	4	7	→	7	4	3	6	21209.18906	-0.00143
8	3	5	8	→	7	3	4	7	22081.81342	-0.00023
8	3	5	9	→	7	3	4	8	22081.97696	0.00171
8	3	5	7	→	7	3	4	6	22081.97696	-0.00102

9	3	7	9	→	8	3	6	8	22519.23883	-0.00076
9	3	7	8	→	8	3	6	7	22519.32759	0.00172
9	3	7	10	→	8	3	6	9	22519.32759	-0.00136
10	2	9	10	→	9	2	8	9	22957.79988	0.00043
10	2	9	11	→	9	2	8	10	22957.82657	0.00073
11	1	11	10	→	10	1	10	9	22970.51058	-0.00115
11	1	11	11	→	10	1	10	10	22970.51058	-0.00119
11	1	11	12	→	10	1	10	11	22970.52588	0.00291
11	0	11	10	→	10	0	10	9	22971.44915	-0.00137
11	0	11	11	→	10	0	10	10	22971.44915	-0.00161
11	0	11	12	→	10	0	10	11	22971.46516	0.00337
10	1	9	10	→	9	1	8	9	23036.90272	-0.00051
10	1	9	9	→	9	1	8	8	23036.90272	-0.00168
10	1	9	11	→	9	1	8	10	23036.91790	0.00145
9	4	6	9	→	8	4	5	8	23282.68542	0.00090
9	4	6	10	→	8	4	5	9	23282.87879	-0.00039
9	4	6	8	→	8	4	5	7	23282.89473	0.00171
9	2	7	8	→	8	2	6	7	23546.51059	0.00036
9	2	7	10	→	8	2	6	9	23546.53080	0.00073
9	2	7	9	→	8	2	6	8	23546.55135	-0.00154
9	4	5	9	→	8	4	4	8	24277.14024	0.00118
9	4	5	10	→	8	4	4	9	24277.38536	0.00067
9	4	5	8	→	8	4	4	7	24277.40251	-0.00048
10	3	8	10	→	9	3	7	9	24728.36485	-0.00206
10	3	8	9	→	9	3	7	8	24728.41737	-0.00123
10	3	8	11	→	9	3	7	10	24728.42639	0.00212
9	3	6	9	→	8	3	5	8	24895.52780	-0.00161
9	3	6	8	→	8	3	5	7	24895.60570	-0.00183
12	1	12	12	→	11	1	11	11	24967.78088	-0.00226
12	1	12	11	→	11	1	11	10	24967.78088	-0.00237
12	1	12	13	→	11	1	11	12	24967.79463	0.00190
12	0	12	12	→	11	0	11	11	24968.13194	-0.00245
12	0	12	11	→	11	0	11	10	24968.13194	-0.00249

Table III(B). Microwave transitions of the $^{13}C_1$ isotopologue of 2FBN in MHz

J'	$K_{a'}$	$K_{c'}$	F'	→	J"	$K_{a"}$	$K_{c"}$	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
3	1	3	3	→	2	1	2	2	6692.91526	0.00034
3	1	3	4	→	2	1	2	3	6693.27229	0.00043
3	0	3	2	→	2	0	2	1	7100.79991	-0.00066
3	0	3	4	→	2	0	2	3	7101.07178	0.00096
3	0	3	3	→	2	0	2	2	7101.08540	-0.00240
3	1	2	3	→	2	1	1	2	8217.84685	0.00022
3	1	2	4	→	2	1	1	3	8218.19763	-0.00044
4	1	4	4	→	3	1	3	3	8822.09975	-0.00017
4	1	4	3	→	3	1	3	2	8822.19318	0.00042
4	1	4	5	→	3	1	3	4	8822.24729	0.00012
4	0	4	3	→	3	0	3	2	9122.00987	-0.00011
4	0	4	5	→	3	0	3	4	9122.13332	0.00059
4	0	4	4	→	3	0	3	3	9122.14779	-0.00041
4	2	3	4	→	3	2	2	3	9948.09425	0.00089
4	2	3	5	→	3	2	2	4	9948.64961	0.00017
4	2	3	3	→	3	2	2	2	9948.79257	0.00027
4	1	3	4	→	3	1	2	3	10780.60620	0.00041
4	1	3	3	→	3	1	2	2	10780.66314	-0.00018
4	1	3	5	→	3	1	2	4	10780.73043	0.00045
4	2	2	4	→	3	2	1	3	10863.56780	-0.00004
4	2	2	5	→	3	2	1	4	10864.17074	0.00034
4	2	2	3	→	3	2	1	2	10864.31320	-0.00068
5	1	5	5	→	4	1	4	4	10899.50651	0.00119
5	1	5	4	→	4	1	4	3	10899.53156	-0.00165
5	1	5	6	→	4	1	4	5	10899.57949	0.00036
5	0	5	4	→	4	0	4	3	11071.82581	-0.00083
5	0	5	6	→	4	0	4	5	11071.89286	-0.00049
5	0	5	5	→	4	0	4	4	11071.89286	0.00208
5	2	4	5	→	4	2	3	4	12293.37086	0.00126
5	2	4	6	→	4	2	3	5	12293.64682	0.00053
5	2	4	4	→	4	2	3	3	12293.67049	-0.00236
6	1	6	6	→	5	1	5	5	12939.54520	-0.00157
6	1	6	5	→	5	1	5	4	12939.55678	0.00223
6	0	6	5	→	5	0	5	4	13023.94332	0.00034
6	0	6	6	→	5	0	5	5	13023.96908	-0.00125
6	0	6	7	→	5	0	5	6	13023.98477	0.00024
5	3	2	5	→	4	3	1	4	13116.99216	-0.00120
5	3	2	6	→	4	3	1	5	13117.68775	0.00062

5	3	2	4	→	4	3	1	3	13117.85180	0.00027
5	1	4	4	→	4	1	3	3	13155.12218	-0.00108
5	1	4	5	→	4	1	3	4	13155.15178	0.00093
5	1	4	6	→	4	1	3	5	13155.18093	0.00047

Table III(C). Microwave transitions of the $^{13}C_2$ isotopologue of 2FBN in MHz

J'	$K_{a'}$	$K_{c'}$	F'	→	J"	$K_{a"}$	$K_{c"}$	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
3	1	3	3	→	2	1	2	2	6689.63540	0.00065
3	1	3	4	→	2	1	2	3	6689.99236	0.00021
3	0	3	4	→	2	0	2	3	7096.37044	0.00047
3	0	3	3	→	2	0	2	2	7096.38788	0.00018
3	1	2	3	→	2	1	1	2	8218.89197	-0.00036
3	1	2	2	→	2	1	1	1	8219.22096	0.00010
3	1	2	4	→	2	1	1	3	8219.24323	-0.00079
4	1	4	4	→	3	1	3	3	8816.78019	-0.00090
4	1	4	3	→	3	1	3	2	8816.87309	-0.00076
4	1	4	5	→	3	1	3	4	8816.92789	-0.00051
4	0	4	3	→	3	0	3	2	9113.89521	-0.00057
4	0	4	5	→	3	0	3	4	9114.01821	-0.00035
4	0	4	4	→	3	0	3	3	9114.03516	0.00100
4	2	3	4	→	3	2	2	3	9946.71606	0.00096
4	2	3	5	→	3	2	2	4	9947.27244	0.00043
4	2	3	3	→	3	2	2	2	9947.41374	-0.00135
4	1	3	4	→	3	1	2	3	10779.55937	-0.00043
4	1	3	3	→	3	1	2	2	10779.61644	0.00000
4	1	3	5	→	3	1	2	4	10779.68368	0.00027
4	2	2	5	→	3	2	1	4	10870.55036	-0.00190
4	2	2	3	→	3	2	1	2	10870.69884	0.00302
5	1	5	5	→	4	1	4	4	10891.94322	0.00141
5	1	5	4	→	4	1	4	3	10891.96811	-0.00150
5	1	5	6	→	4	1	4	5	10892.01613	0.00051
5	0	5	4	→	4	0	4	3	11061.54718	0.00087
5	0	5	6	→	4	0	4	5	11061.61203	-0.00096
5	0	5	5	→	4	0	4	4	11061.61203	0.00191
5	2	4	5	→	4	2	3	4	12290.03450	-0.00055
5	2	4	6	→	4	2	3	5	12290.31263	0.00069
5	2	4	4	→	4	2	3	3	12290.33721	-0.00129
6	1	6	6	→	5	1	5	5	12929.78130	-0.00254
6	1	6	5	→	5	1	5	4	12929.79273	0.00114
6	0	6	5	→	5	0	5	4	13012.32778	0.00135
6	0	6	6	→	5	0	5	5	13012.35277	-0.00067
6	0	6	7	→	5	0	5	6	13012.36844	0.00047
5	3	2	6	→	4	3	1	5	13125.12856	0.00025
5	1	4	4	→	4	1	3	3	13149.49681	0.00004
5	1	4	5	→	4	1	3	4	13149.52520	-0.00041
5	1	4	6	→	4	1	3	5	13149.55461	0.00038

Table III(D). Microwave transitions of the $^{13}C_3$ isotopologue of 2FBN in MHz

J'	$K_{a'}$	$K_{c'}$	F'	→	J"	$K_{a"}$	$K_{c"}$	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
3	1	3	3	→	2	1	2	2	6652.37469	0.00083
3	1	3	4	→	2	1	2	3	6652.73278	0.00082
3	1	2	3	→	2	1	1	2	8166.71792	0.00082
3	1	2	2	→	2	1	1	1	8167.04656	0.00062
3	1	2	4	→	2	1	1	3	8167.06967	-0.00023
4	1	4	4	→	3	1	3	3	8768.92841	0.00003
4	1	4	3	→	3	1	3	2	8769.02131	-0.00014
4	1	4	5	→	3	1	3	4	8769.07596	0.00014
4	0	4	3	→	3	0	3	2	9067.72384	-0.00028
4	0	4	5	→	3	0	3	4	9067.84733	-0.00026
4	0	4	4	→	3	0	3	3	9067.86483	0.00032
4	2	3	4	→	3	2	2	3	9886.90211	0.00046
4	2	3	5	→	3	2	2	4	9887.46088	0.00093
4	2	3	3	→	3	2	2	2	9887.60251	-0.00088
4	1	3	4	→	3	1	2	3	10714.17183	-0.00117
4	1	3	3	→	3	1	2	2	10714.22959	-0.00016
4	1	3	5	→	3	1	2	4	10714.29693	-0.00027
4	2	2	4	→	3	2	1	3	10794.64782	-0.00132
4	2	2	5	→	3	2	1	4	10795.25517	-0.00036
4	2	2	3	→	3	2	1	2	10795.40065	0.00092
5	1	5	5	→	4	1	4	4	10834.07888	0.00120
5	1	5	4	→	4	1	4	3	10834.10350	-0.00189
5	1	5	6	→	4	1	4	5	10834.15192	0.00057
5	0	5	4	→	4	0	4	3	11006.05622	-0.00173
5	0	5	6	→	4	0	4	5	11006.12411	-0.00087
5	0	5	5	→	4	0	4	4	11006.12411	0.00062
5	2	4	5	→	4	2	3	4	12218.18784	0.00031
5	2	4	6	→	4	2	3	5	12218.46598	0.00092
5	2	4	4	→	4	2	3	3	12218.48943	-0.00225
6	1	6	6	→	5	1	5	5	12862.08076	-0.00155
6	1	6	5	→	5	1	5	4	12862.09170	0.00189
6	0	6	5	→	5	0	5	4	12946.45478	0.00126
6	0	6	6	→	5	0	5	5	12946.48029	-0.00142
6	0	6	7	→	5	0	5	6	12946.49600	0.00078
5	3	2	6	→	4	3	1	5	13034.56141	0.00113
5	3	2	4	→	4	3	1	3	13034.72464	-0.00086
5	1	4	4	→	4	1	3	3	13075.20939	0.00163
5	1	4	5	→	4	1	3	4	13075.23696	0.00024
5	1	4	6	→	4	1	3	5	13075.26518	-0.00039

Table III(E). Microwave transitions of the $^{13}C_4$ isotopologue of 2FBN in MHz

J'	$K_{a'}$	$K_{c'}$	F'	→	J"	$K_{a"}$	$K_{c"}$	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
3	1	3	4	→	2	1	2	3	6616.98772	0.00129
3	0	3	4	→	2	0	2	3	7025.02536	0.00020
3	0	3	3	→	2	0	2	2	7025.03886	-0.00139
3	1	2	3	→	2	1	1	2	8102.75830	0.00152
3	1	2	4	→	2	1	1	3	8103.11039	0.00038
4	1	4	4	→	3	1	3	3	8725.68852	-0.00036
4	1	4	3	→	3	1	3	2	8725.78248	-0.00018
4	1	4	5	→	3	1	3	4	8725.83725	0.00042
4	0	4	3	→	3	0	3	2	9033.25787	0.00034
4	0	4	5	→	3	0	3	4	9033.38199	0.00022
4	0	4	4	→	3	0	3	3	9033.39809	0.00070
4	2	3	4	→	3	2	2	3	9819.95351	-0.00019
4	2	3	5	→	3	2	2	4	9820.51262	0.00172
4	2	3	3	→	3	2	2	2	9820.65125	-0.00281
4	1	3	4	→	3	1	2	3	10639.47790	-0.00083
4	1	3	3	→	3	1	2	2	10639.54017	0.00057
4	1	3	5	→	3	1	2	4	10639.60658	0.00070
4	2	2	5	→	3	2	1	4	10691.23714	-0.00106
4	2	2	3	→	3	2	1	2	10691.38156	-0.00102
5	1	5	5	→	4	1	4	4	10784.57151	0.00130
5	1	5	4	→	4	1	4	3	10784.59667	-0.00185
5	1	5	6	→	4	1	4	5	10784.64493	0.00055
5	0	5	4	→	4	0	4	3	10966.23456	0.00029
5	0	5	6	→	4	0	4	5	10966.30119	-0.00046
5	0	5	5	→	4	0	4	4	10966.30119	0.00029
5	2	4	5	→	4	2	3	4	12141.74365	-0.00008
5	2	4	6	→	4	2	3	5	12142.02152	-0.00017
5	2	4	4	→	4	2	3	3	12142.04495	-0.00350
6	1	6	6	→	5	1	5	5	12806.44708	-0.00177
6	1	6	5	→	5	1	5	4	12806.45798	0.00133
6	0	6	5	→	5	0	5	4	12897.83723	0.00093
6	0	6	6	→	5	0	5	5	12897.86462	-0.00108
6	0	6	7	→	5	0	5	6	12897.87934	0.00108
5	3	2	5	→	4	3	1	4	12910.15651	-0.00078
5	3	2	6	→	4	3	1	5	12910.84913	0.00057
5	3	2	4	→	4	3	1	3	12911.01546	0.00277
5	1	4	4	→	4	1	3	3	13000.75389	-0.00087
5	1	4	5	→	4	1	3	4	13000.77941	0.00111
5	1	4	6	→	4	1	3	5	13000.81201	0.00041

Table IIIF. Microwave transitions of the $^{13}C_5$ isotopologue of 2FBN in MHz

J'	K_a'	K_c'	F'	→	J"	K_a"	K_c"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
3	1	3	3	→	2	1	2	2	6631.70847	0.00064
3	1	3	4	→	2	1	2	3	6632.06168	-0.00083
3	0	3	2	→	2	0	2	1	7035.69022	0.00187
3	0	3	4	→	2	0	2	3	7035.95806	0.00124
3	1	2	3	→	2	1	1	2	8143.43673	-0.00093
3	1	2	4	→	2	1	1	3	8143.78651	-0.00032
4	1	4	4	→	3	1	3	3	8741.27673	-0.00008
4	1	4	3	→	3	1	3	2	8741.36876	-0.00029
4	1	4	5	→	3	1	3	4	8741.42323	0.00006
4	0	4	3	→	3	0	3	2	9038.05886	-0.00121
4	0	4	5	→	3	0	3	4	9038.18220	0.00023
4	0	4	4	→	3	0	3	3	9038.19764	0.00054
4	2	3	4	→	3	2	2	3	9857.63000	-0.00030
4	2	3	5	→	3	2	2	4	9858.18307	0.00029
4	2	3	3	→	3	2	2	2	9858.32471	-0.00002
4	1	3	4	→	3	1	2	3	10682.64224	0.00007
4	1	3	3	→	3	1	2	2	10682.69962	0.00020
4	1	3	5	→	3	1	2	4	10682.76512	-0.00045
4	2	2	4	→	3	2	1	3	10765.92919	-0.00004
4	2	2	5	→	3	2	1	4	10766.52768	0.00002
4	2	2	3	→	3	2	1	2	10766.67078	0.00060
5	1	5	5	→	4	1	4	4	10799.50552	0.00025
5	1	5	4	→	4	1	4	3	10799.53118	-0.00184
5	1	5	6	→	4	1	4	5	10799.57850	-0.00018
5	0	5	4	→	4	0	4	3	10969.86746	0.00056
5	0	5	6	→	4	0	4	5	10969.93207	-0.00109
5	0	5	5	→	4	0	4	4	10969.93207	0.00169
5	2	4	5	→	4	2	3	4	12181.34266	-0.00064
5	2	4	6	→	4	2	3	5	12181.61877	0.00055
5	2	4	4	→	4	2	3	3	12181.64249	-0.00213
6	1	6	6	→	5	1	5	5	12820.71248	-0.00227
6	1	6	5	→	5	1	5	4	12820.72451	0.00197
6	0	6	5	→	5	0	5	4	12904.07476	0.00082
6	0	6	6	→	5	0	5	5	12904.10085	-0.00010
6	0	6	7	→	5	0	5	6	12904.11582	0.00059
5	3	2	5	→	4	3	1	4	12999.05801	0.00016
5	3	2	6	→	4	3	1	5	12999.74842	0.00134
5	3	2	4	→	4	3	1	3	12999.90992	-0.00048

5	1	4	4	→	4	1	3	3	13034.95026	-0.00110
5	1	4	5	→	4	1	3	4	13034.97958	0.00092
5	1	4	6	→	4	1	3	5	13035.00853	0.00039

Table III(G). Microwave transitions of the $^{13}C_6$ isotopologue of 2FBN in MHz

J'	K_a'	K_c'	F'	→	J"	K_a"	K_c"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
3	1	3	3	→	2	1	2	2	6671.76071	0.00008
3	1	3	4	→	2	1	2	3	6672.11680	0.00052
3	0	3	4	→	2	0	2	3	7074.54313	0.00070
3	0	3	3	→	2	0	2	2	7074.56108	0.00006
3	1	2	3	→	2	1	1	2	8208.42322	0.00014
3	1	2	4	→	2	1	1	3	8208.77217	-0.00032
4	1	4	4	→	3	1	3	3	8790.94431	0.00023
4	1	4	3	→	3	1	3	2	8791.03545	-0.00056
4	1	4	5	→	3	1	3	4	8791.09060	0.00007
4	0	4	3	→	3	0	3	2	9081.21986	-0.00051
4	0	4	5	→	3	0	3	4	9081.34143	-0.00076
4	0	4	4	→	3	0	3	3	9081.35791	0.00065
4	2	3	4	→	3	2	2	3	9928.06948	-0.00010
4	2	3	5	→	3	2	2	4	9928.62400	0.00018
4	2	3	3	→	3	2	2	2	9928.76457	-0.00165
4	1	3	4	→	3	1	2	3	10760.22099	-0.00069
4	1	3	3	→	3	1	2	2	10760.27895	0.00259
4	1	3	5	→	3	1	2	4	10760.34304	-0.00019
5	1	5	5	→	4	1	4	4	10857.77132	0.00106
5	1	5	4	→	4	1	4	3	10857.79577	-0.00201
5	1	5	6	→	4	1	4	5	10857.84370	0.00002
4	2	2	4	→	3	2	1	3	10867.54552	-0.00091
4	2	2	5	→	3	2	1	4	10868.14722	0.00068
4	2	2	3	→	3	2	1	2	10868.28866	-0.00038
5	0	5	4	→	4	0	4	3	11021.01324	0.00006
5	0	5	6	→	4	0	4	5	11021.07790	-0.00135
5	0	5	5	→	4	0	4	4	11021.07790	0.00265
5	2	4	5	→	4	2	3	4	12263.23890	0.00105
5	2	4	6	→	4	2	3	5	12263.51431	0.00126
5	2	4	4	→	4	2	3	3	12263.53853	-0.00088
6	1	6	6	→	5	1	5	5	12887.45477	-0.00183
6	1	6	5	→	5	1	5	4	12887.46648	0.00210
6	0	6	5	→	5	0	5	4	12965.76571	0.00079
6	0	6	6	→	5	0	5	5	12965.78895	-0.00171
6	0	6	7	→	5	0	5	6	12965.80689	0.00080
5	1	4	4	→	4	1	3	3	13115.86666	-0.00164
5	1	4	5	→	4	1	3	4	13115.89891	-0.00017
5	1	4	6	→	4	1	3	5	13115.92622	0.00053

5	3	2	5	→	4	3	1	4	13121.23427	-0.00020
5	3	2	6	→	4	3	1	5	13121.92999	0.00088
5	3	2	4	→	4	3	1	3	13122.09300	-0.00043

Table III(H). Microwave transitions of the $^{13}C_7$ isotopologue of 2FBN in MHz

J'	K_a'	K_c'	F'	→	J"	K_a"	K_c"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
3	0	3	2	→	2	0	2	1	7050.58484	0.00147
3	0	3	4	→	2	0	2	3	7050.85418	0.00017
3	0	3	3	→	2	0	2	2	7050.86919	-0.00142
3	1	2	3	→	2	1	1	2	8144.98783	0.00012
3	1	2	2	→	2	1	1	1	8145.31851	0.00118
3	1	2	4	→	2	1	1	3	8145.34011	-0.00057
4	1	4	4	→	3	1	3	3	8758.60520	0.00006
4	1	4	3	→	3	1	3	2	8758.69881	0.00024
4	1	4	5	→	3	1	3	4	8758.75296	0.00013
4	0	4	3	→	3	0	3	2	9062.30950	-0.00099
4	0	4	5	→	3	0	3	4	9062.43484	0.00067
4	0	4	4	→	3	0	3	3	9062.44990	-0.00056
4	2	3	4	→	3	2	2	3	9865.94845	0.00019
4	2	3	5	→	3	2	2	4	9866.50613	0.00024
4	2	3	3	→	3	2	2	2	9866.64848	-0.00068
4	1	3	4	→	3	1	2	3	10690.44173	0.00087
4	1	3	3	→	3	1	2	2	10690.49871	-0.00107
4	1	3	5	→	3	1	2	4	10690.56748	0.00089
4	2	2	4	→	3	2	1	3	10755.90956	-0.00075
4	2	2	5	→	3	2	1	4	10756.51549	0.00001
4	2	2	3	→	3	2	1	2	10756.65913	-0.00062
5	1	5	5	→	4	1	4	4	10823.32850	0.00155
5	1	5	4	→	4	1	4	3	10823.35253	-0.00245
5	1	5	6	→	4	1	4	5	10823.40204	0.00116
5	0	5	4	→	4	0	4	3	11000.45877	0.00072
5	0	5	6	→	4	0	4	5	11000.52437	-0.00088
5	0	5	5	→	4	0	4	4	11000.52437	0.00025
5	2	4	5	→	4	2	3	4	12195.53917	0.00021
5	2	4	6	→	4	2	3	5	12195.81749	0.00082
5	2	4	4	→	4	2	3	3	12195.84129	-0.00207
6	1	6	6	→	5	1	5	5	12850.91676	-0.00105
6	1	6	5	→	5	1	5	4	12850.92684	0.00137
6	0	6	5	→	5	0	5	4	12938.93722	0.00027
6	0	6	6	→	5	0	5	5	12938.96495	-0.00078
6	0	6	7	→	5	0	5	6	12938.97891	0.00014
5	3	2	5	→	4	3	1	4	12987.90038	-0.00046
5	3	2	6	→	4	3	1	5	12988.59555	0.00054
5	3	2	4	→	4	3	1	3	12988.76043	0.00080

5	1	4	4	→	4	1	3	3	13054.87707	-0.00119
5	1	4	5	→	4	1	3	4	13054.90575	0.00139
5	1	4	6	→	4	1	3	5	13054.93545	-0.00010

Table III(I). Microwave transitions of the ^{15}N isotopologue of 2FBN in MHz

J'	$K_{a'}$	$K_{c'}$	→	J"	$K_{a"}$	$K_{c"}$	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	1	4	→	3	1	3	8654.55771	0.00062
4	0	4	→	3	0	3	8964.58562	-0.00040
4	2	3	→	3	2	2	9731.36118	-0.00059
4	1	3	→	3	1	2	10541.89651	0.00031
5	1	5	→	4	1	4	10698.48865	0.00020
5	0	5	→	4	0	4	10883.93060	-0.00061
5	2	4	→	4	2	3	12034.89119	0.00063
6	1	6	→	5	1	5	12705.75512	-0.00019
6	0	6	→	5	0	5	12800.19931	0.00025
5	1	4	→	4	1	3	12889.36679	0.00018
5	2	3	→	4	2	2	13405.74187	-0.00030
6	2	5	→	5	2	4	14262.42713	-0.00009

Appendix IV. Microwave transitions of the 3-fluorobenzonitrile (3FBN) and its isotopologues

Table IV(A). Microwave transitions of the parent 3FBN in MHz

J'	$K_{a'}$	$K_{c'}$	F'	→	J"	$K_{a"}$	$K_{c"}$	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
5	1	4	4	→	5	0	5	4	5392.32817	-0.00015
5	1	4	6	→	5	0	5	6	5392.36221	-0.00060
5	1	4	5	→	5	0	5	5	5392.53837	-0.00068
3	1	3	3	→	2	1	2	2	5715.89227	0.00012
3	1	3	2	→	2	1	2	1	5716.20931	0.00217
3	1	3	4	→	2	1	2	3	5716.22290	-0.00020
5	2	3	4	→	5	1	4	4	5869.27798	-0.00067
5	2	3	6	→	5	1	4	6	5869.34455	-0.00036
5	2	3	5	→	5	1	4	5	5869.66963	-0.00068
6	2	4	5	→	6	1	5	5	5936.56422	-0.00009
6	2	4	7	→	6	1	5	7	5936.60089	-0.00036
6	2	4	6	→	6	1	5	6	5936.81964	-0.00051
2	1	2	1	→	1	0	1	0	6023.35268	0.00074
4	2	2	3	→	4	1	3	3	6023.81037	-0.00024
4	2	2	5	→	4	1	3	5	6023.94114	-0.00068
4	2	2	4	→	4	1	3	4	6024.45169	-0.00061
2	1	2	3	→	1	0	1	2	6024.65773	0.00044
2	1	2	2	→	1	0	1	1	6025.12630	0.00121
3	0	3	2	→	2	0	2	1	6077.31319	-0.00013
3	0	3	3	→	2	0	2	2	6077.50087	0.00039
3	0	3	4	→	2	0	2	3	6077.54261	0.00022
3	2	2	3	→	2	2	1	2	6195.08037	0.00044
3	2	2	4	→	2	2	1	3	6196.26688	0.00061
3	2	2	2	→	2	2	1	1	6196.92640	0.00068
7	2	5	6	→	7	1	6	6	6294.69821	0.00003
7	2	5	8	→	7	1	6	8	6294.71989	-0.00039
7	2	5	7	→	7	1	6	7	6294.87345	-0.00022
4	0	4	4	→	3	1	3	3	6413.33281	0.00017
4	0	4	3	→	3	1	3	2	6413.59890	0.00128
4	0	4	5	→	3	1	3	4	6413.61511	-0.00015
6	1	5	5	→	6	0	6	5	6858.45312	0.00055
6	1	5	7	→	6	0	6	7	6858.47695	-0.00019
6	1	5	6	→	6	0	6	6	6858.62184	-0.00055
8	2	6	7	→	8	1	7	7	6995.09505	0.00110
8	2	6	9	→	8	1	7	9	6995.10754	-0.00049
8	2	6	8	→	8	1	7	8	6995.21929	-0.00021
4	1	4	4	→	3	1	3	4	7589.36306	-0.00092
4	1	4	4	→	3	1	3	3	7590.33416	-0.00025
4	1	4	3	→	3	1	3	2	7590.42900	-0.00053
4	1	4	5	→	3	1	3	4	7590.48209	0.00023

4	1	4	3	→	3	1	3	3	7591.73902	-0.00101
3	1	3	3	→	2	0	2	3	7639.25254	-0.00019
3	1	3	2	→	2	0	2	1	7639.90405	-0.00040
3	1	3	4	→	2	0	2	3	7640.22342	0.00026
3	1	3	3	→	2	0	2	2	7640.43768	0.00002
3	1	3	2	→	2	0	2	2	7641.74784	-0.00031
4	0	4	4	→	3	0	3	4	7975.04208	-0.00090
4	0	4	3	→	3	0	3	2	7976.18846	-0.00030
4	0	4	4	→	3	0	3	3	7976.26930	-0.00051
4	0	4	5	→	3	0	3	4	7976.29640	0.00037
4	0	4	3	→	3	0	3	3	7977.84462	-0.00067
9	2	7	8	→	9	1	8	8	8069.50309	-0.00237
9	2	7	10	→	9	1	8	10	8069.51626	0.00132
9	2	7	9	→	9	1	8	9	8069.59915	-0.00045
6	1	5	6	→	5	2	4	5	8116.55609	0.00037
6	1	5	7	→	5	2	4	6	8116.93341	0.00010
6	1	5	5	→	5	2	4	4	8116.97041	0.00015
4	2	3	4	→	3	2	2	3	8237.50502	-0.00060
4	2	3	5	→	3	2	2	4	8238.00798	-0.00006
4	2	3	3	→	3	2	2	2	8238.13598	-0.00064
4	3	2	4	→	3	3	1	3	8315.52771	0.00008
4	3	2	5	→	3	3	1	4	8316.62723	0.00157
4	3	2	3	→	3	3	1	2	8317.05134	0.00033
4	3	1	4	→	3	3	0	3	8326.54811	0.00005
4	3	1	5	→	3	3	0	4	8327.64766	0.00094
4	3	1	3	→	3	3	0	2	8328.07201	-0.00020
4	2	2	4	→	3	2	1	3	8522.47300	-0.00016
4	2	2	5	→	3	2	1	4	8522.97847	0.00053
4	2	2	3	→	3	2	1	2	8523.10686	-0.00043
7	1	6	6	→	7	0	7	6	8597.13186	0.00144
7	1	6	8	→	7	0	7	8	8597.14826	-0.00107
7	1	6	7	→	7	0	7	7	8597.28056	0.00048
5	0	5	5	→	4	1	4	4	8618.71018	0.00017
5	0	5	4	→	4	1	4	3	8618.83557	0.00028
5	0	5	6	→	4	1	4	5	8618.86528	0.00033
10	3	7	9	→	10	2	8	9	8903.05801	0.00015
10	3	7	11	→	10	2	8	11	8903.07176	-0.00007
10	3	7	10	→	10	2	8	10	8903.21077	-0.00021
9	3	6	8	→	9	2	7	8	9090.23744	0.00001
9	3	6	10	→	9	2	7	10	9090.25771	-0.00067
9	3	6	9	→	9	2	7	9	9090.44571	-0.00024
4	1	4	3	→	3	0	3	2	9153.01984	-0.00083
4	1	4	5	→	3	0	3	4	9153.16263	0.00000
4	1	4	4	→	3	0	3	3	9153.27128	-0.00030
5	1	5	5	→	4	1	4	5	9441.88842	-0.00088
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5	1	5	4	→	4	1	4	3	9443.04284	-0.00169
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5	2	4	5	→	5	1	5	5	9474.15353	-0.00030
8	3	5	7	→	8	2	6	7	9516.32963	-0.00104
8	3	5	9	→	8	2	6	9	9516.36262	0.00030
8	3	5	8	→	8	2	6	8	9516.61351	-0.00028
10	2	8	9	→	10	1	9	9	9517.77190	-0.00243
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10	2	8	10	→	10	1	9	10	9517.85016	0.00030
12	3	9	11	→	12	2	10	11	9576.97441	-0.00200
12	3	9	13	→	12	2	10	13	9576.98399	0.00130
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5	0	5	5	→	4	0	4	5	9794.45818	-0.00054
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5	0	5	5	→	4	0	4	4	9795.71223	0.00045
5	0	5	6	→	4	0	4	5	9795.73158	0.00003
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7	3	4	6	→	7	2	5	6	10070.08334	0.00060
7	3	4	8	→	7	2	5	8	10070.13044	-0.00093
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5	2	4	5	→	4	2	3	5	10259.15750	-0.00054
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5	2	4	4	→	4	2	3	4	10260.58101	-0.00122
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5	3	3	5	→	4	3	2	4	10411.67150	-0.00071
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5	3	3	4	→	4	3	2	3	10412.37954	-0.00022
5	3	2	5	→	4	3	1	4	10449.72874	-0.00034
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6	2	5	5	→	6	1	6	5	10457.29388	0.00127
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8	1	7	7	→	8	0	8	7	10526.56322	0.00106
8	1	7	9	→	8	0	8	9	10526.57690	-0.00102
8	1	7	8	→	8	0	8	8	10526.70294	-0.00025
5	1	5	4	→	4	0	4	3	10619.87655	0.00011
5	1	5	6	→	4	0	4	5	10619.95466	0.00017
5	1	5	5	→	4	0	4	4	10620.00930	0.00035
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6	3	3	7	→	6	2	4	7	10635.33698	0.00012
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7	1	6	7	→	6	2	5	6	10886.10601	-0.00061
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6	4	3	6	→	5	4	2	5	12492.82066	-0.00022
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7	3	5	6	→	7	2	6	6	12660.94068	-0.00090
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7	3	5	7	→	7	2	6	7	12661.33821	0.00011
7	0	7	7	→	6	1	6	6	12746.50209	0.00009
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3	2	2	4	→	2	1	1	3	12801.77920	0.00053
3	2	2	3	→	2	1	1	2	12802.32634	0.00074
8	2	7	7	→	8	1	8	7	12886.08882	-0.00115
8	2	7	9	→	8	1	8	9	12886.11768	0.00032
8	2	7	8	→	8	1	8	8	12886.33419	-0.00069
6	1	5	6	→	5	1	4	6	13021.37018	-0.00091
6	1	5	6	→	5	1	4	5	13022.46739	-0.00029
6	1	5	5	→	5	1	4	4	13022.48509	0.00116
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7	1	7	7	→	6	1	6	6	13084.85248	-0.00052
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7	1	7	8	→	6	1	6	7	13084.88664	-0.00023
6	2	4	6	→	5	2	3	5	13089.61743	-0.00009
6	2	4	5	→	5	2	3	4	13089.77035	0.00076
6	2	4	7	→	5	2	3	6	13089.77035	-0.00032
8	3	6	7	→	8	2	7	7	13187.53647	-0.00030
8	3	6	9	→	8	2	7	9	13187.57127	0.00036
8	3	6	8	→	8	2	7	8	13187.84252	0.00038
7	0	7	6	→	6	0	6	5	13288.24888	-0.00025

7	0	7	7	→	6	0	6	6	13288.26335	-0.00007
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8	1	7	8	→	7	2	6	7	13603.04152	-0.00005
8	1	7	9	→	7	2	6	8	13603.21477	0.00147
8	1	7	7	→	7	2	6	6	13603.21477	-0.00146
7	1	7	6	→	6	0	6	5	13626.57665	0.00079
7	1	7	8	→	6	0	6	7	13626.60758	-0.00089
7	1	7	7	→	6	0	6	6	13626.61505	0.00063
3	2	1	2	→	2	1	2	1	13873.82533	0.00127
3	2	1	4	→	2	1	2	3	13874.17910	0.00067
3	2	1	3	→	2	1	2	2	13874.81231	-0.00212
9	3	7	8	→	9	2	8	8	13875.65846	-0.00039
9	3	7	10	→	9	2	8	10	13875.68292	-0.00037
9	3	7	9	→	9	2	8	9	13875.90262	0.00064
7	2	6	7	→	6	2	5	6	14226.97189	-0.00062
7	2	6	6	→	6	2	5	5	14227.06209	-0.00216
7	2	6	8	→	6	2	5	7	14227.07346	0.00094
9	2	8	8	→	9	1	9	8	14298.03612	0.00041
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7	4	3	6	→	6	4	2	5	14614.12613	-0.00135
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8	0	8	7	→	7	1	7	6	14676.14972	-0.00020
8	0	8	9	→	7	1	7	8	14676.16906	0.00013
7	3	4	7	→	6	3	3	6	14819.64831	-0.00030
7	3	4	8	→	6	3	3	7	14819.86476	0.00036
7	3	4	6	→	6	3	3	5	14819.88433	0.00032
8	1	8	8	→	7	1	7	7	14879.36100	-0.00051
8	1	8	7	→	7	1	7	6	14879.36551	-0.00009
8	1	8	9	→	7	1	7	8	14879.38616	0.00015
8	0	8	7	→	7	0	7	6	15014.47443	-0.00222
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8	0	8	9	→	7	0	7	8	15014.49976	0.00104
7	1	6	7	→	6	1	5	6	15026.92026	-0.00086
7	1	6	6	→	6	1	5	5	15026.92772	0.00074
7	1	6	8	→	6	1	5	7	15026.95064	-0.00022
8	1	8	7	→	7	0	7	6	15217.69250	0.00018
8	1	8	8	→	7	0	7	7	15217.71167	-0.00084

8	1	8	9	→	7	0	7	8	15217.71639	0.00059
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7	2	5	6	→	6	2	4	5	15385.06004	-0.00081
7	2	5	8	→	6	2	4	7	15385.07120	0.00131
5	2	4	4	→	4	1	3	3	15850.19344	0.00023
5	2	4	6	→	4	1	3	5	15850.29912	-0.00008
5	2	4	5	→	4	1	3	4	15850.55200	-0.00028
8	2	7	8	→	7	2	6	7	16165.90172	0.00029
8	2	7	7	→	7	2	6	6	16165.95800	-0.00171
8	2	7	9	→	7	2	6	8	16165.97056	0.00075
9	1	8	9	→	8	2	7	8	16208.40762	-0.00023
9	1	8	8	→	8	2	7	7	16208.52442	0.00108
9	1	8	10	→	8	2	7	9	16208.52442	-0.00121
9	0	9	9	→	8	1	8	8	16542.67614	-0.00046
9	0	9	8	→	8	1	8	7	16542.68692	0.00173
9	0	9	10	→	8	1	8	9	16542.70046	-0.00052
9	1	9	9	→	8	1	8	8	16661.19902	0.00044
9	1	9	8	→	8	1	8	7	16661.19902	-0.00179
9	1	9	10	→	8	1	8	9	16661.21799	0.00075
8	5	4	8	→	7	5	3	7	16669.90929	0.00081
8	5	4	9	→	7	5	3	8	16670.29781	0.00151
8	5	4	7	→	7	5	3	6	16670.35367	0.00048
8	5	3	8	→	7	5	2	7	16670.84575	0.00003
8	5	3	9	→	7	5	2	8	16671.23401	0.00044
8	5	3	7	→	7	5	2	6	16671.29056	0.00009
4	2	2	3	→	3	1	3	2	16680.72409	-0.00012
4	2	2	5	→	3	1	3	4	16680.93355	0.00027
4	2	2	4	→	3	1	3	3	16681.39581	0.00037
8	3	6	8	→	7	3	5	7	16692.40584	0.00038
8	3	6	9	→	7	3	5	8	16692.54871	-0.00047
8	3	6	7	→	7	3	5	6	16692.55696	0.00207
8	4	5	8	→	7	4	4	7	16721.91270	0.00068
8	4	5	9	→	7	4	4	8	16722.16394	0.00067
8	4	5	7	→	7	4	4	6	16722.19190	0.00046
9	0	9	8	→	8	0	8	7	16745.89982	-0.00104
9	0	9	9	→	8	0	8	8	16745.90648	0.00171
9	0	9	10	→	8	0	8	9	16745.91744	-0.00062
8	4	4	8	→	7	4	3	7	16751.66664	0.00014
8	4	4	9	→	7	4	3	8	16751.91900	0.00045
8	4	4	7	→	7	4	3	6	16751.94672	-0.00010
9	1	9	8	→	8	0	8	7	16864.41700	0.00052
9	1	9	9	→	8	0	8	8	16864.42487	-0.00188
9	1	9	10	→	8	0	8	9	16864.43513	0.00081
8	1	7	8	→	7	1	6	7	16943.90815	0.00069
8	1	7	7	→	7	1	6	6	16943.90815	-0.00024
8	1	7	9	→	7	1	6	8	16943.92711	-0.00021

8	3	5	8	→	7	3	4	7	17090.39855	0.00013
8	3	5	9	→	7	3	4	8	17090.54555	-0.00048
8	3	5	7	→	7	3	4	6	17090.55372	0.00162
6	2	5	5	→	5	1	4	4	17163.03893	0.00010
6	2	5	7	→	5	1	4	6	17163.10714	0.00045
6	2	5	6	→	5	1	4	5	17163.28268	0.00051
8	2	6	8	→	7	2	5	7	17644.25204	-0.00125
8	2	6	7	→	7	2	5	6	17644.30582	0.00165
8	2	6	9	→	7	2	5	8	17644.31570	0.00063
3	3	0	4	→	2	2	1	3	17995.33356	0.00198
3	3	0	2	→	2	2	1	1	17995.45317	0.00057
3	3	0	3	→	2	2	1	2	17995.68483	0.00223
9	2	8	9	→	8	2	7	8	18073.10743	-0.00006
9	2	8	8	→	8	2	7	7	18073.14671	0.00016
9	2	8	10	→	8	2	7	9	18073.15657	0.00006
10	0	10	10	→	9	1	9	9	18366.38150	-0.00081
10	0	10	9	→	9	1	9	8	18366.38617	-0.00068
10	0	10	11	→	9	1	9	10	18366.40104	0.00100
7	2	6	6	→	6	1	5	5	18367.61856	-0.00059
7	2	6	8	→	6	1	5	7	18367.66477	-0.00011
7	2	6	7	→	6	1	5	6	18367.78682	-0.00018
10	1	10	10	→	9	1	9	9	18433.96116	0.00104
10	1	10	9	→	9	1	9	8	18433.96116	-0.00029
10	1	10	11	→	9	1	9	10	18433.97368	-0.00125
10	0	10	9	→	9	0	9	8	18484.90380	0.00133
10	0	10	10	→	9	0	9	9	18484.90380	-0.00049
10	0	10	11	→	9	0	9	10	18484.91537	-0.00093
10	1	10	9	→	9	0	9	8	18552.47527	-0.00180
10	1	10	10	→	9	0	9	9	18552.48320	0.00110
10	1	10	11	→	9	0	9	10	18552.49169	0.00049
10	1	9	10	→	9	2	8	9	18660.21750	-0.00140
10	1	9	9	→	9	2	8	8	18660.29446	-0.00040
10	1	9	11	→	9	2	8	10	18660.30098	0.00137
9	3	7	9	→	8	3	6	8	18761.16676	-0.00057
9	3	7	8	→	8	3	6	7	18761.26858	-0.00005
9	3	7	10	→	8	3	6	9	18761.26858	-0.00030
9	1	8	8	→	8	1	7	7	18771.26780	0.00098
9	1	8	9	→	8	1	7	8	18771.26780	0.00009
9	1	8	10	→	8	1	7	9	18771.28156	-0.00058
9	4	6	9	→	8	4	5	8	18848.58322	0.00037
9	4	6	10	→	8	4	5	9	18848.76150	0.00055
9	4	6	8	→	8	4	5	7	18848.77364	-0.00097
9	4	5	9	→	8	4	4	8	18917.97749	0.00011
9	4	5	10	→	8	4	4	9	18918.15617	-0.00074
9	4	5	8	→	8	4	4	7	18918.17222	0.00150
9	3	6	9	→	8	3	5	8	19419.47975	-0.00021

9	3	6	8	→	8	3	5	7	19419.58526	0.00017
9	3	6	10	→	8	3	5	9	19419.58526	0.00015
8	2	7	7	→	7	1	6	6	19506.65210	0.00023
8	2	7	9	→	7	1	6	8	19506.68290	-0.00093
8	2	7	8	→	7	1	6	7	19506.76745	0.00014
9	2	7	9	→	8	2	6	8	19845.64808	0.00028
9	2	7	8	→	8	2	6	7	19845.67642	-0.00192
9	2	7	10	→	8	2	6	9	19845.68969	0.00063
5	2	3	4	→	4	1	4	3	19880.44279	0.00054
5	2	3	6	→	4	1	4	5	19880.57257	-0.00011
5	2	3	5	→	4	1	4	4	19880.91946	0.00009
10	2	9	10	→	9	2	8	9	19949.31181	0.00084
10	2	9	9	→	9	2	8	8	19949.33647	-0.00187
10	2	9	11	→	9	2	8	10	19949.34851	0.00098
4	3	2	3	→	3	2	1	2	19965.13288	0.00123
4	3	2	5	→	3	2	1	4	19965.24677	0.00073
4	3	2	4	→	3	2	1	3	19965.68873	-0.00045
4	3	1	3	→	3	2	2	2	20126.59963	0.00054
4	3	1	5	→	3	2	2	4	20126.71304	0.00102
4	3	1	4	→	3	2	2	3	20127.15087	0.00014
11	0	11	11	→	10	1	10	10	20162.75088	-0.00026
11	0	11	10	→	10	1	10	9	20162.75088	-0.00278
11	0	11	12	→	10	1	10	11	20162.76626	0.00149
11	1	11	11	→	10	1	10	10	20200.60387	-0.00066
11	1	11	10	→	10	1	10	9	20200.60387	-0.00157
11	1	11	12	→	10	1	10	11	20200.61782	0.00114
11	0	11	10	→	10	0	10	9	20230.32744	-0.00082
11	0	11	11	→	10	0	10	10	20230.32744	-0.00151
11	0	11	12	→	10	0	10	11	20230.34121	0.00155
11	1	11	10	→	10	0	10	9	20268.18050	0.00047
11	1	11	11	→	10	0	10	10	20268.18050	-0.00185
11	1	11	12	→	10	0	10	11	20268.19248	0.00090
10	1	9	9	→	9	1	8	8	20524.91739	-0.00067
10	1	9	10	→	9	1	8	9	20524.91739	-0.00115
10	1	9	11	→	9	1	8	10	20524.93248	0.00199
9	2	8	8	→	8	1	7	7	20635.88955	-0.00048
9	2	8	10	→	8	1	7	9	20635.91369	0.00066
9	2	8	9	→	8	1	7	8	20635.96648	-0.00086
10	3	8	10	→	9	3	7	9	20805.88608	-0.00055
10	3	8	9	→	9	3	7	8	20805.96078	0.00287
10	3	8	11	→	9	3	7	10	20805.96078	-0.00007
11	1	10	11	→	10	2	9	10	20945.42176	0.00038
11	1	10	10	→	10	2	9	9	20945.46981	-0.00130
11	1	10	12	→	10	2	9	11	20945.47717	0.00029
10	4	6	10	→	9	4	5	9	21123.09954	0.00109
10	4	6	11	→	9	4	5	10	21123.23155	0.00005

10	4	6	9	→	9	4	5	8	21123.23909	0.00124
10	3	7	10	→	9	3	6	9	21785.93250	-0.00134
10	3	7	9	→	9	3	6	8	21786.01041	0.00305
10	3	7	11	→	9	3	6	10	21786.01041	0.00016
11	2	10	11	→	10	2	9	10	21796.96632	-0.00078
11	2	10	10	→	10	2	9	9	21796.98569	-0.00138
11	2	10	12	→	10	2	9	11	21796.99623	0.00090
10	2	9	9	→	9	1	8	8	21813.96098	-0.00056
10	2	9	11	→	9	1	8	10	21813.97875	0.00033
10	2	9	10	→	9	1	8	9	21814.01025	-0.00036
5	3	3	4	→	4	2	2	3	21854.40431	0.00019
5	3	3	6	→	4	2	2	5	21854.50861	-0.00004
5	3	3	5	→	4	2	2	4	21854.88742	-0.00081
12	0	12	12	→	11	1	11	11	21942.43160	-0.00067
12	0	12	11	→	11	1	11	10	21942.43160	-0.00218
12	0	12	13	→	11	1	11	12	21942.44437	0.00114
12	1	12	12	→	11	1	11	11	21963.33367	-0.00113
12	1	12	11	→	11	1	11	10	21963.33367	-0.00184
12	1	12	13	→	11	1	11	12	21963.34643	0.00141
10	2	8	10	→	9	2	7	9	21973.16817	-0.00063
10	2	8	9	→	9	2	7	8	21973.18584	-0.00109
10	2	8	11	→	9	2	7	10	21973.19806	0.00126
12	0	12	11	→	11	0	11	10	21980.28433	-0.00123
12	0	12	12	→	11	0	11	11	21980.28433	-0.00133
12	0	12	13	→	11	0	11	12	21980.29658	0.00144
12	1	12	11	→	11	0	11	10	22001.18602	-0.00126
12	1	12	12	→	11	0	11	11	22001.18602	-0.00218
12	1	12	13	→	11	0	11	12	22001.19769	0.00076
11	1	10	11	→	10	1	9	10	22234.51299	-0.00047
11	1	10	10	→	10	1	9	9	22234.51299	-0.00161
11	1	10	12	→	10	1	9	11	22234.52645	0.00165
5	3	2	4	→	4	2	3	3	22338.90162	0.00094
5	3	2	6	→	4	2	3	5	22339.00357	0.00082
5	3	2	5	→	4	2	3	4	22339.37356	-0.00063
6	3	4	5	→	5	2	3	4	23575.13353	-0.00121
6	3	4	7	→	5	2	3	6	23575.21304	-0.00082
6	3	4	6	→	5	2	3	5	23575.52306	0.00005
13	0	13	13	→	12	1	12	12	23712.26132	-0.00093
13	0	13	12	→	12	1	12	11	23712.26132	-0.00194
13	0	13	14	→	12	1	12	13	23712.27370	0.00232
13	1	13	13	→	12	1	12	12	23723.66821	-0.00128
13	1	13	12	→	12	1	12	11	23723.66821	-0.00189
13	1	13	14	→	12	1	12	13	23723.67901	0.00077
13	0	13	13	→	12	0	12	12	23733.16396	-0.00083
13	0	13	12	→	12	0	12	11	23733.16396	-0.00102
13	0	13	14	→	12	0	12	13	23733.17612	0.00295

13	1	13	12	→	12	0	12	11	23744.56980	-0.00202
13	1	13	13	→	12	0	12	12	23744.56980	-0.00223
13	1	13	14	→	12	0	12	13	23744.58142	0.00139
12	1	11	12	→	11	1	10	11	23929.87150	-0.00042
12	1	11	11	→	11	1	10	10	23929.87150	-0.00343
12	1	11	13	→	11	1	10	12	23929.88530	0.00190

Table IV(B). Microwave transitions of the $^{13}C_1$ isotopologue of 3FBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	1	4	4	→	3	1	3	3	7578.20806	-0.00018
4	1	4	3	→	3	1	3	2	7578.30278	-0.00064
4	1	4	5	→	3	1	3	4	7578.35619	0.00036
4	0	4	3	→	3	0	3	2	7963.58687	-0.00061
4	0	4	4	→	3	0	3	3	7963.66769	-0.00056
4	0	4	5	→	3	0	3	4	7963.69524	0.00049
5	0	5	4	→	4	0	4	3	9780.91927	-0.00023
5	0	5	5	→	4	0	4	4	9780.96367	0.00008
5	0	5	6	→	4	0	4	5	9780.98371	0.00029
5	2	4	5	→	4	2	3	4	10241.84549	0.00057
5	2	4	6	→	4	2	3	5	10242.10897	0.00075
5	2	4	4	→	4	2	3	3	10242.13555	0.00028
5	1	5	4	→	4	0	4	3	10609.50590	-0.00023
5	1	5	6	→	4	0	4	5	10609.58498	0.00084
5	1	5	5	→	4	0	4	4	10609.63679	-0.00130
6	0	6	6	→	5	1	5	5	10710.84672	0.00034
6	0	6	5	→	5	1	5	4	10710.90943	-0.00015
6	0	6	7	→	5	1	5	6	10710.93647	0.00020
5	2	3	5	→	4	2	2	4	10768.47606	-0.00049
5	2	3	6	→	4	2	2	5	10768.73964	0.00028
5	2	3	4	→	4	2	2	3	10768.76418	-0.00150
5	1	4	5	→	4	1	3	4	10924.89354	0.00047
5	1	4	4	→	4	1	3	3	10924.93298	0.00048
5	1	4	6	→	4	1	3	5	10924.97162	0.00054
6	1	6	6	→	5	1	5	5	11256.37548	0.00069
6	1	6	5	→	5	1	5	4	11256.39102	-0.00052
6	1	6	7	→	5	1	5	6	11256.42391	-0.00105
6	0	6	5	→	5	0	5	4	11539.49538	-0.00084
6	0	6	6	→	5	0	5	5	11539.52193	0.00104
6	0	6	7	→	5	0	5	6	11539.53663	-0.00036
6	1	6	5	→	5	0	5	4	12084.97767	-0.00051
6	1	6	7	→	5	0	5	6	12085.02720	0.00152
6	1	6	6	→	5	0	5	5	12085.04924	-0.00005
6	2	5	6	→	5	2	4	5	12236.40124	0.00108
6	2	5	5	→	5	2	4	4	12236.55615	0.00091
6	2	5	7	→	5	2	4	6	12236.55615	0.00041
6	1	5	6	→	5	1	4	5	12999.72793	0.00073
6	1	5	5	→	5	1	4	4	12999.74102	-0.00267
6	1	5	7	→	5	1	4	6	12999.77443	0.00038
6	2	4	6	→	5	2	3	5	13063.57231	-0.00042
6	2	4	5	→	5	2	3	4	13063.72583	0.00110
6	2	4	7	→	5	2	3	6	13063.72583	0.00002

7	1	7	7	→	6	1	6	6	13064.83874	-0.00111
7	1	7	6	→	6	1	6	5	13064.84839	0.00046
7	1	7	8	→	6	1	6	7	13064.87400	0.00017
7	1	7	6	→	6	0	6	5	13610.33010	0.00021
7	1	7	8	→	6	0	6	7	13610.36116	-0.00135
7	1	7	7	→	6	0	6	6	13610.36938	0.00113

Table IV(C). Microwave transitions of the $^{13}C_2$ isotopologue of 3FBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	1	4	4	→	3	1	3	3	7582.50697	-0.00022
4	1	4	3	→	3	1	3	2	7582.60235	-0.00018
4	1	4	5	→	3	1	3	4	7582.65510	0.00003
4	0	4	3	→	3	0	3	2	7967.55937	-0.00033
4	0	4	4	→	3	0	3	3	7967.64067	-0.00021
4	0	4	5	→	3	0	3	4	7967.66768	0.00043
5	0	5	4	→	4	0	4	3	9783.14014	-0.00202
5	0	5	5	→	4	0	4	4	9783.18600	0.00123
5	0	5	6	→	4	0	4	5	9783.20149	-0.00024
5	2	4	5	→	4	2	3	4	10252.86708	0.00066
5	2	4	6	→	4	2	3	5	10253.12853	-0.00005
5	2	4	4	→	4	2	3	3	10253.15150	-0.00137
5	1	5	4	→	4	0	4	3	10591.46584	-0.00129
5	1	5	6	→	4	0	4	5	10591.54824	0.00302
5	1	5	5	→	4	0	4	4	10591.59713	-0.00180
5	1	4	5	→	4	1	3	4	10939.33670	0.00053
5	1	4	4	→	4	1	3	3	10939.37552	0.00000
5	1	4	6	→	4	1	3	5	10939.41484	0.00063
6	1	6	6	→	5	1	5	5	11260.79226	0.00094
6	1	6	5	→	5	1	5	4	11260.80763	-0.00043
6	1	6	7	→	5	1	5	6	11260.84114	-0.00042
6	0	6	5	→	5	0	5	4	11540.16641	0.00148
6	0	6	6	→	5	0	5	5	11540.19193	0.00059
6	0	6	7	→	5	0	5	6	11540.21071	0.00043
6	1	6	5	→	5	0	5	4	12069.13076	-0.00227
6	1	6	7	→	5	0	5	6	12069.18762	0.00257
6	1	6	6	→	5	0	5	5	12069.20512	-0.00036
6	2	5	6	→	5	2	4	5	12248.40532	-0.00005
6	2	5	5	→	5	2	4	4	12248.56117	0.00044
6	2	5	7	→	5	2	4	6	12248.56117	-0.00008
7	0	7	7	→	6	1	6	6	12740.07298	0.00003
7	0	7	6	→	6	1	6	5	12740.10518	0.00028
7	0	7	8	→	6	1	6	7	12740.12802	0.00019
6	1	5	6	→	5	1	4	5	13014.12546	0.00029
6	1	5	5	→	5	1	4	4	13014.13995	-0.00153
6	1	5	7	→	5	1	4	6	13014.17243	0.00050
7	1	7	7	→	6	1	6	6	13068.98548	-0.00224
7	1	7	6	→	6	1	6	5	13068.99620	0.00042
7	1	7	8	→	6	1	6	7	13069.02208	0.00035
7	1	7	6	→	6	0	6	5	13597.96375	-0.00013
7	1	7	8	→	6	0	6	7	13597.99502	-0.00148
7	1	7	7	→	6	0	6	6	13598.00358	0.00173

Table IV(D). Microwave transitions of the $^{13}C_3$ isotopologue of 3FBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	1	4	4	→	3	1	3	3	7561.11046	0.00012
4	1	4	3	→	3	1	3	2	7561.20499	-0.00029
4	1	4	5	→	3	1	3	4	7561.25721	-0.00041
4	0	4	3	→	3	0	3	2	7945.71144	-0.00008
4	0	4	4	→	3	0	3	3	7945.79129	-0.00053
4	0	4	5	→	3	0	3	4	7945.81905	0.00056
5	0	5	4	→	4	0	4	3	9759.43326	-0.00058
5	0	5	5	→	4	0	4	4	9759.47741	-0.00009
5	0	5	6	→	4	0	4	5	9759.49814	0.00072
5	2	4	5	→	4	2	3	4	10217.82130	0.00137
5	2	4	6	→	4	2	3	5	10218.08314	0.00064
5	2	4	4	→	4	2	3	3	10218.10874	-0.00067
5	1	5	4	→	4	0	4	3	10589.85562	-0.00083
5	1	5	6	→	4	0	4	5	10589.93582	0.00163
5	1	5	5	→	4	0	4	4	10589.98728	-0.00025
6	0	6	6	→	5	1	5	5	10684.00832	-0.00022
6	0	6	5	→	5	1	5	4	10684.07184	0.00037
6	0	6	7	→	5	1	5	6	10684.09756	-0.00057
5	2	3	5	→	4	2	2	4	10741.51120	0.00014
5	2	3	6	→	4	2	2	5	10741.77320	0.00019
5	2	3	4	→	4	2	2	3	10741.79917	-0.00008
5	1	4	5	→	4	1	3	4	10898.78672	-0.00055
5	1	4	4	→	4	1	3	3	10898.82609	-0.00066
5	1	4	6	→	4	1	3	5	10898.86552	0.00035
6	1	6	6	→	5	1	5	5	11231.32468	0.00091
6	1	6	5	→	5	1	5	4	11231.33949	-0.00104
6	1	6	7	→	5	1	5	6	11231.37395	0.00007
6	0	6	5	→	5	0	5	4	11514.49381	-0.00027
6	0	6	6	→	5	0	5	5	11514.51817	-0.00040
6	0	6	7	→	5	0	5	6	11514.53496	0.00006
6	1	6	5	→	5	0	5	4	12061.76234	-0.00080
6	1	6	7	→	5	0	5	6	12061.81197	0.00133
6	1	6	6	→	5	0	5	5	12061.83337	-0.00043
6	2	5	6	→	5	2	4	5	12207.89815	-0.00005
6	2	5	5	→	5	2	4	4	12208.05398	0.00104
6	2	5	7	→	5	2	4	6	12208.05398	0.00054
7	0	7	7	→	6	1	6	6	12693.17146	0.00107
7	0	7	6	→	6	1	6	5	12693.20250	-0.00008
7	0	7	8	→	6	1	6	7	12693.22595	0.00057
6	1	5	6	→	5	1	4	5	12969.14917	0.00037
6	1	5	5	→	5	1	4	4	12969.16372	-0.00171
6	1	5	7	→	5	1	4	6	12969.19619	0.00052

6	2	4	6	→	5	2	3	5	13030.78821	-0.00051
6	2	4	5	→	5	2	3	4	13030.94135	0.00114
6	2	4	7	→	5	2	3	6	13030.94135	0.00007
7	1	7	7	→	6	1	6	6	13035.93433	-0.00217
7	1	7	6	→	6	1	6	5	13035.94511	0.00050
7	1	7	8	→	6	1	6	7	13035.97054	0.00009
7	1	7	6	→	6	0	6	5	13583.21384	0.00017
7	1	7	8	→	6	0	6	7	13583.24519	-0.00101
7	1	7	7	→	6	0	6	6	13583.25282	0.00110

Table IV(E). Microwave transitions of the $^{13}C_4$ isotopologue of 3FBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	1	4	4	→	3	1	3	3	7540.00358	-0.00056
4	1	4	3	→	3	1	3	2	7540.09957	-0.00013
4	1	4	5	→	3	1	3	4	7540.15206	0.00012
4	0	4	3	→	3	0	3	2	7923.40949	0.00049
4	0	4	4	→	3	0	3	3	7923.48986	-0.00164
4	0	4	5	→	3	0	3	4	7923.51685	-0.00004
5	0	5	4	→	4	0	4	3	9731.41541	-0.00028
5	0	5	5	→	4	0	4	4	9731.46238	0.00099
5	0	5	6	→	4	0	4	5	9731.48022	0.00013
5	2	4	5	→	4	2	3	4	10190.51691	-0.00098
5	2	4	6	→	4	2	3	5	10190.78333	0.00126
5	2	4	4	→	4	2	3	3	10190.80813	-0.00111
5	1	5	4	→	4	0	4	3	10554.58829	-0.00115
5	1	5	6	→	4	0	4	5	10554.66935	0.00106
5	1	5	5	→	4	0	4	4	10554.72588	0.00010
6	0	6	6	→	5	1	5	5	10657.73868	0.00043
6	0	6	5	→	5	1	5	4	10657.80267	-0.00030
6	0	6	7	→	5	1	5	6	10657.82941	0.00000
5	2	3	5	→	4	2	2	4	10715.08101	0.00151
5	2	3	6	→	4	2	2	5	10715.34511	0.00070
5	2	3	4	→	4	2	2	3	10715.37019	-0.00071
5	1	4	5	→	4	1	3	4	10870.30353	-0.00033
5	1	4	4	→	4	1	3	3	10870.34278	0.00015
5	1	4	6	→	4	1	3	5	10870.38206	0.00034
6	1	6	6	→	5	1	5	5	11199.51349	0.00045
6	1	6	5	→	5	1	5	4	11199.52913	-0.00047
6	1	6	7	→	5	1	5	6	11199.56285	-0.00015
6	0	6	5	→	5	0	5	4	11480.97621	-0.00051
6	0	6	6	→	5	0	5	5	11481.00366	0.00102
6	0	6	7	→	5	0	5	6	11481.01701	-0.00060
6	1	6	5	→	5	0	5	4	12022.70252	-0.00082
6	1	6	7	→	5	0	5	6	12022.75264	0.00143
6	1	6	6	→	5	0	5	5	12022.77771	0.00028
6	2	5	6	→	5	2	4	5	12175.01089	0.00019
6	2	5	5	→	5	2	4	4	12175.16711	0.00106
6	2	5	7	→	5	2	4	6	12175.16711	0.00051
7	0	7	7	→	6	1	6	6	12659.98193	0.00115
7	0	7	6	→	6	1	6	5	12660.01427	0.00046
7	0	7	8	→	6	1	6	7	12660.03695	0.00043
6	1	5	6	→	5	1	4	5	12934.60825	0.00033
6	1	5	5	→	5	1	4	4	12934.62285	-0.00068
6	1	5	7	→	5	1	4	6	12934.65483	0.00056

7	1	7	7	→	6	1	6	6	12998.78209	-0.00284
7	1	7	6	→	6	1	6	5	12998.79222	-0.00052
7	1	7	8	→	6	1	6	7	12998.81918	0.00054
6	2	4	6	→	5	2	3	5	12998.81940	0.00010
6	2	4	5	→	5	2	3	4	12998.97161	-0.00112
6	2	4	7	→	5	2	3	6	12998.97161	-0.00220
7	1	7	6	→	6	0	6	5	13540.51960	0.00024
7	1	7	8	→	6	0	6	7	13540.55137	-0.00087
7	1	7	7	→	6	0	6	6	13540.56060	0.00088

Table IV(F). Microwave transitions of the $^{13}C_5$ isotopologue of 3FBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	1	4	4	→	3	1	3	3	7549.17218	-0.00040
4	1	4	3	→	3	1	3	2	7549.26821	0.00027
4	1	4	5	→	3	1	3	4	7549.32036	-0.00007
4	0	4	3	→	3	0	3	2	7931.11631	-0.00057
4	0	4	4	→	3	0	3	3	7931.19788	-0.00141
4	0	4	5	→	3	0	3	4	7931.22448	-0.00026
5	0	5	4	→	4	0	4	3	9732.48189	0.00011
5	0	5	5	→	4	0	4	4	9732.52618	-0.00026
5	0	5	6	→	4	0	4	5	9732.54470	-0.00014
5	2	4	5	→	4	2	3	4	10219.39558	0.00055
5	2	4	6	→	4	2	3	5	10219.65921	0.00063
5	2	4	4	→	4	2	3	3	10219.68461	-0.00046
5	1	5	4	→	4	0	4	3	10492.59307	-0.00045
5	1	5	6	→	4	0	4	5	10492.67328	0.00157
5	1	5	5	→	4	0	4	4	10492.72626	0.00025
6	0	6	6	→	5	1	5	5	10716.06266	0.00079
6	0	6	5	→	5	1	5	4	10716.12424	0.00028
6	0	6	7	→	5	1	5	6	10716.15109	0.00022
5	2	3	6	→	4	2	2	5	10776.77327	0.00004
5	2	3	4	→	4	2	2	3	10776.79798	-0.00164
5	1	4	5	→	4	1	3	4	10909.46179	0.00077
5	1	4	4	→	4	1	3	3	10909.50091	0.00122
5	1	4	6	→	4	1	3	5	10909.53964	0.00099
6	1	6	6	→	5	1	5	5	11206.84606	0.00095
6	1	6	5	→	5	1	5	4	11206.85968	-0.00197
6	1	6	7	→	5	1	5	6	11206.89517	0.00001
6	0	6	5	→	5	0	5	4	11476.23476	-0.00094
6	0	6	6	→	5	0	5	5	11476.26307	0.00163
6	0	6	7	→	5	0	5	6	11476.27748	-0.00026
6	1	6	5	→	5	0	5	4	11966.97238	-0.00101
6	1	6	7	→	5	0	5	6	11967.02406	0.00203
6	1	6	6	→	5	0	5	5	11967.04354	-0.00114
6	2	5	6	→	5	2	4	5	12205.77995	0.00015
6	2	5	5	→	5	2	4	4	12205.93531	0.00021
6	2	5	7	→	5	2	4	6	12205.93531	-0.00034
7	0	7	7	→	6	1	6	6	12703.24881	-0.00007
7	0	7	6	→	6	1	6	5	12703.28020	0.00006
7	0	7	8	→	6	1	6	7	12703.30393	0.00080
6	1	5	6	→	5	1	4	5	12972.15754	-0.00001
6	1	5	5	→	5	1	4	4	12972.17196	-0.00098
6	1	5	7	→	5	1	4	6	12972.20323	-0.00038
7	1	7	7	→	6	1	6	6	13004.19868	-0.00094

7	1	7	6	→	6	1	6	5	13004.20722	-0.00028
7	1	7	8	→	6	1	6	7	13004.23402	0.00057
6	2	4	6	→	5	2	3	5	13074.22998	-0.00093
6	2	4	5	→	5	2	3	4	13074.38497	0.00148
6	2	4	7	→	5	2	3	6	13074.38497	0.00029
7	1	7	6	→	6	0	6	5	13494.94548	0.00028
7	1	7	8	→	6	0	6	7	13494.97614	-0.00161
7	1	7	7	→	6	0	6	6	13494.98383	0.00097

Table IV(G). Microwave transitions of the $^{13}C_6$ isotopologue of 3FBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	1	4	4	→	3	1	3	3	7563.81382	-0.00070
4	1	4	3	→	3	1	3	2	7563.90706	-0.00183
4	1	4	5	→	3	1	3	4	7563.96164	0.00065
4	0	4	3	→	3	0	3	2	7947.30097	0.00060
4	0	4	4	→	3	0	3	3	7947.37968	-0.00115
4	0	4	5	→	3	0	3	4	7947.40708	0.00018
5	0	5	4	→	4	0	4	3	9755.52245	-0.00125
5	0	5	5	→	4	0	4	4	9755.56806	0.00118
5	0	5	6	→	4	0	4	5	9755.58534	-0.00039
5	2	4	5	→	4	2	3	4	10232.96339	0.00189
5	2	4	6	→	4	2	3	5	10233.22327	0.00110
5	2	4	4	→	4	2	3	3	10233.24806	-0.00020
5	1	5	4	→	4	0	4	3	10540.94700	-0.00035
5	1	5	6	→	4	0	4	5	10541.02582	0.00129
5	1	5	5	→	4	0	4	4	10541.07667	-0.00031
6	0	6	6	→	5	1	5	5	10720.14740	0.00056
6	0	6	5	→	5	1	5	4	10720.20809	-0.00021
6	0	6	7	→	5	1	5	6	10720.23568	0.00068
5	2	3	5	→	4	2	2	4	10778.93764	-0.00001
5	2	3	6	→	4	2	2	5	10779.19943	0.00086
5	2	3	4	→	4	2	2	3	10779.22364	-0.00102
5	1	4	5	→	4	1	3	4	10920.83000	-0.00107
5	1	4	4	→	4	1	3	3	10920.86941	-0.00056
5	1	4	6	→	4	1	3	5	10920.90845	0.00017
6	1	6	6	→	5	1	5	5	11230.98576	0.00161
6	1	6	5	→	5	1	5	4	11231.00027	-0.00044
6	1	6	7	→	5	1	5	6	11231.03289	-0.00102
6	0	6	5	→	5	0	5	4	11505.63151	-0.00045
6	0	6	6	→	5	0	5	5	11505.65789	0.00096
6	0	6	7	→	5	0	5	6	11505.67350	-0.00030
6	1	6	5	→	5	0	5	4	12016.42351	-0.00086
6	1	6	7	→	5	0	5	6	12016.47449	0.00178
6	1	6	6	→	5	0	5	5	12016.49370	-0.00055
6	2	5	6	→	5	2	4	5	12223.41651	0.00031
6	2	5	5	→	5	2	4	4	12223.57067	0.00061
6	2	5	7	→	5	2	4	6	12223.57067	0.00010
7	0	7	7	→	6	1	6	6	12717.79037	-0.00065
7	0	7	6	→	6	1	6	5	12717.82221	0.00004
7	0	7	8	→	6	1	6	7	12717.84578	0.00083
6	1	5	6	→	5	1	4	5	12989.17248	-0.00052
6	1	5	5	→	5	1	4	4	12989.18658	-0.00244
6	1	5	7	→	5	1	4	6	12989.21997	0.00079

7	1	7	7	→	6	1	6	6	13033.38449	-0.00133
7	1	7	6	→	6	1	6	5	13033.39261	-0.00120
7	1	7	8	→	6	1	6	7	13033.41980	0.00027
6	2	4	6	→	5	2	3	5	13076.92203	-0.00012
6	2	4	5	→	5	2	3	4	13077.07489	0.00214
6	2	4	7	→	5	2	3	6	13077.07489	0.00100
7	1	7	6	→	6	0	6	5	13544.18697	0.00075
7	1	7	8	→	6	0	6	7	13544.21788	-0.00056
7	1	7	7	→	6	0	6	6	13544.22383	0.00070

Table IV(H). Microwave transitions of the $^{13}C_7$ isotopologue of 3FBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	1	4	4	→	3	1	3	3	7514.35432	-0.00039
4	1	4	3	→	3	1	3	2	7514.44924	-0.00090
4	1	4	5	→	3	1	3	4	7514.50258	0.00017
4	0	4	3	→	3	0	3	2	7897.10252	-0.00038
4	0	4	4	→	3	0	3	3	7897.18475	0.00037
4	0	4	5	→	3	0	3	4	7897.21167	0.00121
5	0	5	4	→	4	0	4	3	9702.69764	-0.00051
5	0	5	5	→	4	0	4	4	9702.74342	0.00066
5	0	5	6	→	4	0	4	5	9702.76172	-0.00003
5	2	4	5	→	4	2	3	4	10148.83333	0.00045
5	2	4	6	→	4	2	3	5	10149.09664	0.00029
5	2	4	4	→	4	2	3	3	10149.12231	-0.00086
5	1	5	4	→	4	0	4	3	10551.63752	-0.00050
5	1	5	6	→	4	0	4	5	10551.71738	0.00074
5	1	5	5	→	4	0	4	4	10551.77254	-0.00066
6	0	6	6	→	5	1	5	5	10600.77158	-0.00049
6	0	6	5	→	5	1	5	4	10600.83648	-0.00046
6	0	6	7	→	5	1	5	6	10600.86351	0.00016
5	2	3	5	→	4	2	2	4	10658.28839	-0.00023
5	2	3	6	→	4	2	2	5	10658.55349	0.00102
5	2	3	4	→	4	2	2	3	10658.57790	-0.00099
5	1	4	5	→	4	1	3	4	10822.14156	-0.00047
5	1	4	4	→	4	1	3	3	10822.18105	-0.00021
5	1	4	6	→	4	1	3	5	10822.22063	0.00054
6	1	6	6	→	5	1	5	5	11164.04580	0.00164
6	1	6	5	→	5	1	5	4	11164.05988	-0.00093
6	1	6	7	→	5	1	5	6	11164.09444	0.00020
6	0	6	5	→	5	0	5	4	11449.77695	0.00014
6	0	6	6	→	5	0	5	5	11449.80291	0.00039
6	0	6	7	→	5	0	5	6	11449.81798	-0.00026
6	1	6	5	→	5	0	5	4	12012.99973	-0.00095
6	1	6	7	→	5	0	5	6	12013.05070	0.00157
6	1	6	6	→	5	0	5	5	12013.07383	-0.00078
6	2	5	6	→	5	2	4	5	12126.74148	0.00105
6	2	5	5	→	5	2	4	4	12126.89661	0.00093
6	2	5	7	→	5	2	4	6	12126.89661	0.00041
7	0	7	7	→	6	1	6	6	12603.74041	0.00065
7	0	7	6	→	6	1	6	5	12603.77296	-0.00016
7	0	7	8	→	6	1	6	7	12603.79601	0.00025
6	1	5	6	→	5	1	4	5	12880.96935	0.00022
6	1	5	5	→	5	1	4	4	12880.98363	-0.00174
6	1	5	7	→	5	1	4	6	12881.01597	0.00006

6	2	4	6	→	5	2	3	5	12929.33590	0.00019
6	2	4	5	→	5	2	3	4	12929.48947	0.00085
6	2	4	7	→	5	2	3	6	12929.48947	-0.00019
7	1	7	7	→	6	1	6	6	12958.93243	-0.00193
7	1	7	6	→	6	1	6	5	12958.94237	0.00001
7	1	7	8	→	6	1	6	7	12958.96834	0.00014
7	1	7	6	→	6	0	6	5	13522.16674	0.00051
7	1	7	8	→	6	0	6	7	13522.19826	-0.00083
7	1	7	7	→	6	0	6	6	13522.20743	0.00098

Table IV(I). Microwave transitions of the ^{15}N isotopologue of 3FBN in MHz

J'	$K_{a'}$	$K_{c'}$	→	J"	$K_{a"}$	$K_{c"}$	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	1	4	→	3	1	3	7424.91475	-0.00011
4	0	4	→	3	0	3	7803.72556	-0.00041
4	2	3	→	3	2	2	8043.12589	-0.00033
4	2	2	→	3	2	1	8303.79844	-0.00055
4	1	3	→	3	1	2	8593.88643	0.00007
4	1	4	→	3	0	3	9030.00396	0.00075
5	1	5	→	4	1	4	9239.73747	-0.00012
5	0	5	→	4	0	4	9592.18409	0.00020
5	2	4	→	4	2	3	10019.76505	0.00009
5	3	3	→	4	3	2	10159.08952	-0.00114
6	0	6	→	5	1	5	10448.78478	0.00022
5	1	5	→	4	0	4	10466.01404	-0.00080
5	2	3	→	4	2	2	10507.55246	0.00036
5	1	4	→	4	1	3	10679.87076	0.00067
6	1	6	→	5	1	5	11034.13732	-0.00002
6	0	6	→	5	0	5	11322.61595	0.00044
6	1	6	→	5	0	5	11907.96858	0.00029
6	2	5	→	5	2	4	11974.18152	0.00000
7	0	7	→	6	1	6	12436.87237	0.00048
6	1	5	→	5	1	4	12715.82356	0.00072
6	2	4	→	5	2	3	12745.50237	0.00026
7	1	7	→	6	1	6	12809.68873	0.00026
7	1	7	→	6	0	6	13395.04067	-0.00058
7	2	6	→	6	2	5	13902.88095	0.00020
8	0	8	→	7	1	7	14340.91990	-0.00014
7	3	4	→	6	3	3	14438.63682	-0.00098

Appendix V. Microwave transitions of the 2,3-difluorobenzonitrile (23DFBN) and its isotopologues

Table V(A). Microwave transitions of the parent 23DFBN in MHz

J'	$K_{a'}$	$K_{c'}$	F'	→	J"	$K_{a"}$	$K_{c"}$	F"	ν_{obs}	$\nu_{obs.-calc.}$
3	2	1	3	→	2	2	0	2	6226.90827	0.00024
3	2	1	4	→	2	2	0	3	6228.19557	0.00106
3	2	1	2	→	2	2	0	1	6228.89327	0.00038
3	1	2	3	→	2	1	1	2	6419.09933	0.00012
3	1	2	2	→	2	1	1	1	6419.41638	-0.00175
3	1	2	4	→	2	1	1	3	6419.42781	0.00057
3	3	1	2	→	3	2	2	2	6455.45925	-0.00022
3	3	1	4	→	3	2	2	4	6456.02004	-0.00053
3	3	1	3	→	3	2	2	3	6457.62247	0.00003
4	0	4	4	→	3	1	3	3	6641.26380	-0.00003
4	0	4	3	→	3	1	3	2	6641.46696	-0.00110
4	0	4	5	→	3	1	3	4	6641.49909	0.00048
4	3	2	3	→	4	2	3	3	6685.44894	0.00011
4	3	2	5	→	4	2	3	5	6685.69523	0.00018
4	3	2	4	→	4	2	3	4	6686.65282	0.00037
8	4	4	7	→	8	3	5	7	6715.17524	-0.00043
8	4	4	9	→	8	3	5	9	6715.22667	-0.00060
8	4	4	8	→	8	3	5	8	6715.63686	-0.00043
4	1	4	4	→	3	1	3	3	6869.30985	0.00001
4	1	4	3	→	3	1	3	2	6869.39796	-0.00023
4	1	4	5	→	3	1	3	4	6869.45255	0.00007
4	0	4	3	→	3	0	3	2	7093.78742	-0.00014
4	0	4	4	→	3	0	3	3	7093.89295	-0.00156
4	0	4	5	→	3	0	3	4	7093.90026	0.00124
5	3	3	4	→	5	2	4	4	7101.02925	-0.00001
5	3	3	6	→	5	2	4	6	7101.15576	-0.00007
5	3	3	5	→	5	2	4	5	7101.77725	0.00006
5	2	4	4	→	5	1	5	4	7109.86194	0.00008
5	2	4	6	→	5	1	5	6	7109.94645	-0.00023
5	2	4	5	→	5	1	5	5	7110.36322	0.00009
4	1	4	3	→	3	0	3	2	7321.71747	-0.00022
4	1	4	5	→	3	0	3	4	7321.85299	0.00010
4	1	4	4	→	3	0	3	3	7321.94029	-0.00023
7	4	3	6	→	7	3	4	6	7378.69828	-0.00025
7	4	3	8	→	7	3	4	8	7378.77960	-0.00050
7	4	3	7	→	7	3	4	7	7379.34547	-0.00031
2	2	1	1	→	1	1	0	1	7555.37060	0.00008
2	2	1	3	→	1	1	0	2	7556.66091	0.00082
2	2	1	1	→	1	1	0	0	7556.87037	0.00218
2	2	1	2	→	1	1	0	1	7557.30550	0.00101

2	2	1	2	→	1	1	0	2	7557.90304	-0.00038
6	1	5	5	→	6	0	6	5	7613.45108	0.00027
6	1	5	7	→	6	0	6	7	7613.47568	-0.00158
6	1	5	6	→	6	0	6	6	7613.63349	-0.00035
6	3	4	5	→	6	2	5	5	7737.68765	-0.00007
6	3	4	7	→	6	2	5	7	7737.75935	-0.00014
6	3	4	6	→	6	2	5	6	7738.18453	-0.00010
4	2	3	4	→	3	2	2	3	7761.70934	0.00003
4	2	3	5	→	3	2	2	4	7762.22756	0.00052
4	2	3	3	→	3	2	2	2	7762.35994	-0.00010
4	3	2	4	→	3	3	1	3	7990.73963	0.00031
4	3	2	5	→	3	3	1	4	7991.90239	0.00087
4	3	2	3	→	3	3	1	2	7992.34966	0.00026
6	4	2	5	→	6	3	3	5	8027.42362	-0.00022
6	4	2	7	→	6	3	3	7	8027.54863	-0.00077
6	4	2	6	→	6	3	3	6	8028.29282	-0.00034
2	2	0	1	→	1	1	1	1	8056.92324	0.00023
2	2	0	3	→	1	1	1	2	8058.15451	0.00075
2	2	0	1	→	1	1	1	0	8058.32754	0.00132
2	2	0	2	→	1	1	1	1	8058.79836	0.00055
2	2	0	2	→	1	1	1	2	8059.35895	-0.00011
4	3	1	4	→	3	3	0	3	8073.47786	0.00069
4	3	1	5	→	3	3	0	4	8074.65963	0.00095
4	3	1	3	→	3	3	0	2	8075.11111	0.00023
6	2	4	6	→	5	3	3	5	8168.48087	0.00075
6	2	4	7	→	5	3	3	6	8169.33505	0.00081
6	2	4	5	→	5	3	3	4	8169.47291	0.00012
5	1	4	5	→	4	2	3	4	8210.12619	0.00005
5	1	4	6	→	4	2	3	5	8210.69967	-0.00021
5	1	4	4	→	4	2	3	3	8210.78945	0.00046
5	0	5	5	→	4	1	4	4	8380.81446	0.00024
5	0	5	4	→	4	1	4	3	8380.88561	-0.00020
5	0	5	6	→	4	1	4	5	8380.92349	0.00001
4	1	3	4	→	3	1	2	4	8411.56012	-0.00103
4	1	3	4	→	3	1	2	3	8412.49056	-0.00010
4	1	3	3	→	3	1	2	2	8412.55662	-0.00134
4	1	3	5	→	3	1	2	4	8412.61322	0.00024
4	1	3	3	→	3	1	2	3	8413.81235	-0.00084
6	2	5	5	→	6	0	6	5	8427.53043	0.00025
6	2	5	7	→	6	0	6	7	8427.58509	-0.00044
6	2	5	6	→	6	0	6	6	8427.91290	-0.00030
5	1	5	5	→	4	1	4	5	8482.38554	-0.00084
5	1	5	5	→	4	1	4	4	8483.50748	0.00049
5	1	5	4	→	4	1	4	3	8483.53678	-0.00011
5	1	5	6	→	4	1	4	5	8483.58201	0.00036
5	1	5	4	→	4	1	4	4	8484.94540	-0.00063

4	2	2	4	→	3	2	1	3	8503.02370	0.00015
4	2	2	5	→	3	2	1	4	8503.56582	0.00034
4	2	2	3	→	3	2	1	2	8503.69780	0.00066
6	3	4	5	→	6	1	5	5	8551.76612	-0.00097
6	3	4	7	→	6	1	5	7	8551.86671	-0.00104
6	3	4	6	→	6	1	5	6	8552.46351	-0.00048
5	0	5	5	→	4	0	4	5	8607.64635	-0.00113
5	0	5	4	→	4	0	4	3	8608.81564	-0.00030
5	0	5	5	→	4	0	4	4	8608.86063	0.00040
5	0	5	6	→	4	0	4	5	8608.87738	0.00002
5	0	5	4	→	4	0	4	4	8610.34035	-0.00060
5	1	5	4	→	4	0	4	3	8711.46669	-0.00034
5	1	5	6	→	4	0	4	5	8711.53578	0.00026
5	1	5	5	→	4	0	4	4	8711.55292	-0.00008
7	3	5	6	→	7	1	6	6	9033.53468	-0.00077
7	3	5	8	→	7	1	6	8	9033.59096	-0.00050
7	3	5	7	→	7	1	6	7	9033.97943	-0.00026
3	2	2	2	→	2	1	1	1	9109.13307	0.00058
3	2	2	4	→	2	1	1	3	9109.46670	-0.00013
3	2	2	3	→	2	1	1	2	9110.06820	-0.00017
7	1	6	6	→	7	0	7	6	9373.79334	0.00118
7	1	6	8	→	7	0	7	8	9373.81643	-0.00140
7	1	6	7	→	7	0	7	7	9373.99567	-0.00002
5	2	4	5	→	4	2	3	5	9585.40678	-0.00092
5	2	4	5	→	4	2	3	4	9585.92560	0.00023
5	2	4	6	→	4	2	3	5	9586.18700	0.00048
5	2	4	4	→	4	2	3	3	9586.21155	-0.00041
5	2	4	4	→	4	2	3	4	9586.86245	-0.00067
8	3	6	7	→	8	1	7	7	9895.80455	-0.00103
8	3	6	9	→	8	1	7	9	9895.83913	0.00001
8	3	6	8	→	8	1	7	8	9896.10537	0.00008
5	3	3	5	→	4	3	2	4	10001.04982	-0.00029
5	3	3	6	→	4	3	2	5	10001.64758	0.00028
5	3	3	4	→	4	3	2	3	10001.79217	-0.00022
5	4	2	5	→	4	4	1	4	10005.54699	0.00033
5	4	2	6	→	4	4	1	5	10006.60491	0.00043
5	4	2	4	→	4	4	1	3	10006.91815	-0.00011
5	4	1	5	→	4	4	0	4	10019.49124	0.00037
5	4	1	6	→	4	4	0	5	10020.55379	0.00140
5	4	1	4	→	4	4	0	3	10020.86635	-0.00056
6	0	6	6	→	5	1	5	5	10025.72660	-0.00038
6	0	6	5	→	5	1	5	4	10025.75233	-0.00067
6	0	6	7	→	5	1	5	6	10025.78562	0.00070
6	1	6	6	→	5	1	5	6	10067.52247	-0.00095
6	1	6	6	→	5	1	5	5	10068.71840	-0.00029
6	1	6	5	→	5	1	5	4	10068.73067	0.00047

6	1	6	7	→	5	1	5	6	10068.76459	0.00036
6	1	6	5	→	5	1	5	5	10070.16842	-0.00081
6	0	6	6	→	5	0	5	6	10127.18877	-0.00111
6	0	6	5	→	5	0	5	4	10128.40529	0.00120
6	0	6	6	→	5	0	5	5	10128.42002	0.00027
6	0	6	7	→	5	0	5	6	10128.44337	0.00028
6	0	6	5	→	5	0	5	5	10129.88414	-0.00066
8	3	5	8	→	7	4	4	7	10150.24419	-0.00005
8	3	5	9	→	7	4	4	8	10150.98701	0.00066
8	3	5	7	→	7	4	4	6	10151.07452	-0.00090
6	1	6	5	→	5	0	5	4	10171.38177	0.00049
6	1	6	6	→	5	0	5	5	10171.41184	0.00038
6	1	6	7	→	5	0	5	6	10171.42266	0.00026
5	1	4	5	→	4	1	3	5	10249.26082	-0.00131
5	1	4	4	→	4	1	3	3	10250.30158	-0.00386
5	1	4	5	→	4	1	3	4	10250.31434	0.00038
5	1	4	6	→	4	1	3	5	10250.35386	0.00033
5	1	4	4	→	4	1	3	4	10251.62698	-0.00099
5	3	2	5	→	4	3	1	4	10266.43557	-0.00035
5	3	2	6	→	4	3	1	5	10267.06725	-0.00016
5	3	2	4	→	4	3	1	3	10267.21830	0.00019
4	2	3	3	→	3	1	2	2	10452.07460	0.00019
4	2	3	5	→	3	1	2	4	10452.26657	-0.00006
4	2	3	4	→	3	1	2	3	10452.67829	-0.00018
6	1	5	6	→	5	2	4	5	10528.99784	0.00015
6	1	5	7	→	5	2	4	6	10529.31608	0.00057
6	1	5	5	→	5	2	4	4	10529.34174	-0.00021
5	2	3	5	→	4	2	2	5	10758.73391	-0.00134
5	2	3	5	→	4	2	2	4	10759.35831	-0.00004
5	2	3	6	→	4	2	2	5	10759.61975	0.00072
5	2	3	4	→	4	2	2	3	10759.63721	-0.00153
5	2	3	4	→	4	2	2	4	10760.42134	-0.00104
3	2	1	2	→	2	1	2	1	10773.76480	0.00085
3	2	1	4	→	2	1	2	3	10774.09339	0.00073
3	2	1	3	→	2	1	2	2	10774.65306	-0.00036
6	2	5	6	→	5	2	4	5	11343.27741	0.00036
6	2	5	5	→	5	2	4	4	11343.42348	0.00216
6	2	5	7	→	5	2	4	6	11343.42348	-0.00029
7	0	7	7	→	6	1	6	6	11619.64335	-0.00092
7	0	7	6	→	6	1	6	5	11619.65531	0.00074
7	0	7	8	→	6	1	6	7	11619.68042	0.00046
5	2	4	4	→	4	1	3	3	11625.72836	-0.00005
5	2	4	6	→	4	1	3	5	11625.84041	0.00024
5	2	4	5	→	4	1	3	4	11626.11286	-0.00032
7	1	7	7	→	6	1	6	6	11636.78704	-0.00114
7	1	7	6	→	6	1	6	5	11636.79431	0.00078

7	1	7	8	→	6	1	6	7	11636.81992	0.00036
7	0	7	6	→	6	0	6	5	11662.63070	-0.00107
7	0	7	7	→	6	0	6	6	11662.63738	0.00140
7	0	7	8	→	6	0	6	7	11662.65924	-0.00003
7	1	7	6	→	6	0	6	5	11679.76963	-0.00110
7	1	7	7	→	6	0	6	6	11679.78172	0.00182
7	1	7	8	→	6	0	6	7	11679.79860	-0.00027
6	1	5	5	→	5	1	4	4	11904.76419	-0.00073
6	1	5	6	→	5	1	4	5	11904.79565	-0.00126
6	1	5	7	→	5	1	4	6	11904.80351	0.00136
6	3	4	6	→	5	3	3	5	11979.68422	-0.00026
6	3	4	7	→	5	3	3	6	11980.02834	0.00090
6	3	4	5	→	5	3	3	4	11980.07892	-0.00087
6	5	2	6	→	5	5	1	5	11997.54908	0.00009
6	5	2	7	→	5	5	1	6	11998.50823	0.00073
6	5	2	5	→	5	5	1	4	11998.73890	-0.00032
6	5	1	6	→	5	5	0	5	11999.52027	-0.00007
6	5	1	7	→	5	5	0	6	12000.47963	0.00025
6	5	1	5	→	5	5	0	4	12000.71066	-0.00052
6	4	3	6	→	5	4	2	5	12059.95550	0.00013
6	4	3	7	→	5	4	2	6	12060.57605	0.00059
6	4	3	5	→	5	4	2	4	12060.70692	-0.00042
6	4	2	6	→	5	4	1	5	12119.86810	0.00023
6	4	2	7	→	5	4	1	6	12120.49869	0.00024
6	4	2	5	→	5	4	1	4	12120.63176	-0.00014
3	3	1	4	→	2	2	0	3	12239.02356	0.00040
3	3	1	2	→	2	2	0	1	12239.13320	0.00113
3	3	1	3	→	2	2	0	2	12239.42057	0.00077
3	3	0	4	→	2	2	1	3	12348.38819	0.00040
3	3	0	2	→	2	2	1	1	12348.52091	0.00079
3	3	0	3	→	2	2	1	2	12348.74038	0.00047
6	3	3	6	→	5	3	2	5	12580.49994	-0.00047
6	3	3	7	→	5	3	2	6	12580.88328	0.00061
6	3	3	5	→	5	3	2	4	12580.93819	-0.00137
7	1	6	7	→	6	2	5	6	12608.71835	-0.00012
7	1	6	8	→	6	2	5	7	12608.89262	0.00105
7	1	6	6	→	6	2	5	5	12608.89262	-0.00113
6	2	5	5	→	5	1	4	4	12718.84427	-0.00002
6	2	5	7	→	5	1	4	6	12718.90996	-0.00045
6	2	5	6	→	5	1	4	5	12719.07597	-0.00030
6	2	4	6	→	5	2	3	5	12910.39929	-0.00013
6	2	4	5	→	5	2	3	4	12910.51629	-0.00158
6	2	4	7	→	5	2	3	6	12910.52788	0.00067
7	2	6	7	→	6	2	5	6	13036.06471	0.00036
7	2	6	6	→	6	2	5	5	13036.14122	-0.00220
7	2	6	8	→	6	2	5	7	13036.15384	0.00046

8	0	8	8	→	7	1	7	7	13189.46530	-0.00077
8	0	8	7	→	7	1	7	6	13189.47235	0.00136
8	0	8	9	→	7	1	7	8	13189.49057	-0.00057
8	1	8	8	→	7	1	7	7	13196.07376	0.00261
8	1	8	7	→	7	1	7	6	13196.07376	-0.00064
8	1	8	9	→	7	1	7	8	13196.09424	-0.00050
8	0	8	7	→	7	0	7	6	13206.61027	0.00032
8	0	8	8	→	7	0	7	7	13206.61027	0.00029
8	0	8	9	→	7	0	7	8	13206.62995	-0.00078
8	1	8	7	→	7	0	7	6	13213.21481	0.00144
8	1	8	8	→	7	0	7	7	13213.21481	-0.00025
8	1	8	9	→	7	0	7	8	13213.23359	-0.00075
7	1	6	6	→	6	1	5	5	13422.97405	0.00093
7	1	6	7	→	6	1	5	6	13422.99862	0.00079
7	1	6	8	→	6	1	5	7	13422.99862	-0.00121
7	2	6	6	→	6	1	5	5	13850.22231	-0.00048
7	2	6	8	→	6	1	5	7	13850.26209	0.00045
7	2	6	7	→	6	1	5	6	13850.34345	-0.00026
8	2	6	8	→	7	3	5	7	13888.58409	0.00033
8	2	6	9	→	7	3	5	8	13888.95305	0.00034
8	2	6	7	→	7	3	5	6	13888.98595	-0.00018
7	3	5	7	→	6	3	4	6	13904.51351	-0.00002
7	3	5	8	→	6	3	4	7	13904.72412	0.00058
7	3	5	6	→	6	3	4	5	13904.74070	-0.00077
4	3	2	3	→	3	2	1	2	14002.58894	0.00036
4	3	2	5	→	3	2	1	4	14002.73030	0.00012
4	3	2	4	→	3	2	1	3	14003.25124	0.00015
7	5	3	7	→	6	5	2	6	14056.38250	0.00031
7	5	3	8	→	6	5	2	7	14056.99458	0.00053
7	5	3	6	→	6	5	2	5	14057.10824	0.00031
7	5	2	7	→	6	5	1	6	14066.89138	0.00047
7	5	2	8	→	6	5	1	7	14067.50506	0.00028
7	5	2	6	→	6	5	1	5	14067.61962	0.00067
7	4	4	7	→	6	4	3	6	14120.20025	-0.00024
7	4	4	8	→	6	4	3	7	14120.59412	0.00032
7	4	4	6	→	6	4	3	5	14120.65359	-0.00080
7	4	3	7	→	6	4	2	6	14304.17874	-0.00062
7	4	3	8	→	6	4	2	7	14304.59531	0.00087
7	4	3	6	→	6	4	2	5	14304.65616	-0.00166
8	1	7	8	→	7	2	6	7	14470.53772	0.00023
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8	1	7	9	→	7	2	6	8	14470.63451	0.00137
4	3	1	3	→	3	2	2	2	14544.91855	0.00011
4	3	1	5	→	3	2	2	4	14545.02592	0.00086
4	3	1	4	→	3	2	2	3	14545.43929	0.00036
8	2	7	8	→	7	2	6	7	14674.89788	-0.00078

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8	2	7	9	→	7	2	6	8	14674.95816	0.00128
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9	0	9	8	→	8	1	8	7	14748.85613	0.00016
9	0	9	10	→	8	1	8	9	14748.87072	-0.00146
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9	1	9	10	→	8	1	8	9	14751.34997	-0.00184
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9	1	9	10	→	8	0	8	9	14757.95383	-0.00159
8	1	7	7	→	7	1	6	6	14897.87476	-0.00151
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8	3	6	8	→	7	3	5	7	15760.00987	0.00090
8	3	6	9	→	7	3	5	8	15760.14324	0.00063
8	3	6	7	→	7	3	5	6	15760.14324	-0.00317
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8	6	2	8	→	7	6	1	7	16042.56421	0.00018
8	6	2	9	→	7	6	1	8	16043.15562	0.00029
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8	4	5	9	→	7	4	4	8	16166.27901	0.00080
8	4	5	7	→	7	4	4	6	16166.30664	-0.00021
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8	5	3	7	→	7	5	2	6	16176.71416	-0.00099
9	1	8	9	→	8	2	7	8	16183.43985	-0.00027
9	1	8	8	→	8	2	7	7	16183.48627	-0.00182

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9	2	8	9	→	8	2	7	8	16274.89532	0.00004
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9	1	8	8	→	8	1	7	7	16387.80843	0.00133
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9	2	7	10	→	8	3	6	9	16426.22288	0.00089
9	2	7	8	→	8	3	6	7	16426.23485	-0.00067
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8	4	4	7	→	7	4	3	6	16606.58727	-0.00011
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6	3	4	7	→	5	2	3	6	16721.21999	-0.00042
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5	3	2	4	→	4	2	3	3	17049.77643	-0.00008
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9	3	7	9	→	8	3	6	8	17539.98639	0.00078
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7	3	5	6	→	6	2	4	5	17715.35009	0.00161
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9	4	5	9	→	8	4	4	8	19021.10640	-0.00038
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11	1	10	10	→	10	2	9	9	19397.17659	-0.00208
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9	3	7	8	→	8	2	6	7	19411.23093	-0.00021
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11	1	10	10	→	10	1	9	9	19436.18986	-0.00262
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12	1	11	12	→	11	2	10	11	20962.90601	0.00134
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13	1	12	13	→	12	2	11	12	22520.15238	0.00185
13	1	12	12	→	12	2	11	11	22520.16177	-0.00186
13	1	12	14	→	12	2	11	13	22520.17123	0.00136
13	2	12	13	→	12	2	11	12	22522.66617	-0.00013
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13	1	12	13	→	12	1	11	12	22526.57897	-0.00085
13	1	12	12	→	12	1	11	11	22526.58982	-0.00215
13	1	12	14	→	12	1	11	13	22526.59993	0.00165
13	2	12	13	→	12	1	11	12	22529.09568	0.00009
13	2	12	12	→	12	1	11	11	22529.10553	-0.00186
13	2	12	14	→	12	1	11	13	22529.11514	0.00141

Table V(B). Microwave transitions of the $^{13}C_1$ isotopologue of 23DFBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	1	4	4	→	3	1	3	3	6858.88044	0.00017
4	1	4	3	→	3	1	3	2	6858.96789	-0.00068
4	1	4	5	→	3	1	3	4	6859.02272	-0.00012
4	0	4	3	→	3	0	3	2	7083.69607	-0.00032
4	0	4	4	→	3	0	3	3	7083.80124	-0.00130
4	0	4	5	→	3	0	3	4	7083.80858	0.00099
4	1	4	3	→	3	0	3	2	7312.82561	-0.00091
4	2	3	4	→	3	2	2	3	7748.72904	-0.00024
4	2	3	5	→	3	2	2	4	7749.24645	0.00049
4	2	3	3	→	3	2	2	2	7749.37863	-0.00006
5	0	5	5	→	4	1	4	4	8367.45340	0.00024
5	0	5	4	→	4	1	4	3	8367.52363	-0.00116
5	0	5	6	→	4	1	4	5	8367.56288	0.00045
4	1	3	4	→	3	1	2	3	8398.34121	0.00028
4	1	3	3	→	3	1	2	2	8398.40981	0.00095
4	1	3	5	→	3	1	2	4	8398.46363	0.00014
5	1	5	5	→	4	1	4	4	8470.88219	-0.00023
5	1	5	4	→	4	1	4	3	8470.91298	0.00056
5	1	5	6	→	4	1	4	5	8470.95711	-0.00003
5	0	5	4	→	4	0	4	3	8596.65492	-0.00001
5	0	5	5	→	4	0	4	4	8596.69962	0.00076
5	0	5	6	→	4	0	4	5	8596.71620	-0.00005
5	1	5	4	→	4	0	4	3	8700.04285	0.00029
5	1	5	6	→	4	0	4	5	8700.11110	0.00015
5	1	5	5	→	4	0	4	4	8700.12720	-0.00093
6	0	6	6	→	5	1	5	5	10010.55156	-0.00009
6	0	6	5	→	5	1	5	4	10010.57689	-0.00090
6	0	6	7	→	5	1	5	6	10010.60957	-0.00011
6	0	6	5	→	5	0	5	4	10113.96777	0.00235
6	0	6	6	→	5	0	5	5	10113.98289	0.00197
6	0	6	7	→	5	0	5	6	10114.00225	-0.00213
6	1	6	5	→	5	0	5	4	10157.33089	-0.00129
6	1	6	6	→	5	0	5	5	10157.36145	-0.00075
6	1	6	7	→	5	0	5	6	10157.37515	0.00190
5	2	3	5	→	4	2	2	4	10739.33063	0.00034
5	2	3	6	→	4	2	2	5	10739.59096	0.00057
5	2	3	4	→	4	2	2	3	10739.60741	-0.00276
6	2	5	6	→	5	2	4	5	11325.36716	0.00027
6	2	5	5	→	5	2	4	4	11325.51319	0.00202
6	2	5	7	→	5	2	4	6	11325.51319	-0.00038
7	0	7	7	→	6	1	6	6	11602.49516	0.00022
7	0	7	6	→	6	1	6	5	11602.50613	0.00079

7	0	7	8	→	6	1	6	7	11602.53069	-0.00002
7	0	7	6	→	6	0	6	5	11645.87124	-0.00085
7	0	7	7	→	6	0	6	6	11645.87753	0.00131
7	0	7	8	→	6	0	6	7	11645.89888	-0.00070
7	1	7	6	→	6	0	6	5	11663.19777	-0.00068
7	1	7	7	→	6	0	6	6	11663.20886	0.00132
7	1	7	8	→	6	0	6	7	11663.22614	-0.00044
7	1	6	7	→	6	2	5	6	12585.35458	0.00002
7	1	6	8	→	6	2	5	7	12585.52821	0.00054
7	1	6	6	→	6	2	5	5	12585.52821	-0.00166
6	2	5	5	→	5	1	4	4	12706.25778	-0.00052
6	2	5	7	→	5	1	4	6	12706.32406	-0.00006
6	2	5	6	→	5	1	4	5	12706.48899	0.00022
6	2	4	6	→	5	2	3	5	12887.48724	0.00046
6	2	4	5	→	5	2	3	4	12887.60426	-0.00114
6	2	4	7	→	5	2	3	6	12887.61632	0.00173
7	2	6	7	→	6	2	5	6	13016.06111	-0.00074
7	2	6	6	→	6	2	5	5	13016.14116	0.00010
7	2	6	8	→	6	2	5	7	13016.15129	0.00031
8	0	8	8	→	7	1	7	7	13170.21516	-0.00136
8	0	8	7	→	7	1	7	6	13170.22259	0.00107
8	0	8	9	→	7	1	7	8	13170.24206	0.00041
8	1	8	8	→	7	1	7	7	13176.90677	0.00068
8	1	8	7	→	7	1	7	6	13176.90677	-0.00264
8	1	8	9	→	7	1	7	8	13176.92943	-0.00031
8	1	8	7	→	7	0	7	6	13194.23670	0.00093
8	1	8	8	→	7	0	7	7	13194.23670	-0.00071
8	1	8	9	→	7	0	7	8	13194.25709	0.00036

Table V(C). Microwave transitions of the $^{13}C_2$ isotopologue of 23DFBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	1	4	4	→	3	1	3	3	6866.48705	0.00011
4	1	4	3	→	3	1	3	2	6866.57523	0.00004
4	1	4	5	→	3	1	3	4	6866.62934	-0.00013
4	0	4	3	→	3	0	3	2	7090.05163	-0.00054
4	0	4	4	→	3	0	3	3	7090.15820	-0.00099
4	0	4	5	→	3	0	3	4	7090.16519	0.00161
4	1	4	3	→	3	0	3	2	7316.03597	0.00063
4	1	4	5	→	3	0	3	4	7316.17060	0.00019
4	1	4	4	→	3	0	3	3	7316.25831	0.00045
4	2	3	4	→	3	2	2	3	7759.95617	0.00024
4	2	3	5	→	3	2	2	4	7760.47406	0.00053
4	2	3	3	→	3	2	2	2	7760.60659	0.00010
5	0	5	5	→	4	1	4	4	8378.13028	0.00022
5	0	5	4	→	4	1	4	3	8378.19782	-0.00353
5	0	5	6	→	4	1	4	5	8378.23951	0.00047
4	1	3	4	→	3	1	2	3	8410.67924	-0.00024
4	1	3	3	→	3	1	2	2	8410.74612	-0.00023
4	1	3	5	→	3	1	2	4	8410.80149	0.00002
5	1	5	5	→	4	1	4	4	8479.71278	-0.00042
5	1	5	4	→	4	1	4	3	8479.74326	0.00023
5	1	5	6	→	4	1	4	5	8479.78796	0.00019
5	0	5	4	→	4	0	4	3	8604.18465	0.00014
5	0	5	5	→	4	0	4	4	8604.22952	0.00080
5	0	5	6	→	4	0	4	5	8604.24586	-0.00002
5	1	5	4	→	4	0	4	3	8705.72669	0.00049
5	1	5	6	→	4	0	4	5	8705.79554	0.00094
5	1	5	5	→	4	0	4	4	8705.81073	-0.00113
6	0	6	6	→	5	1	5	5	10021.54864	0.00096
6	0	6	5	→	5	1	5	4	10021.57295	-0.00061
6	0	6	7	→	5	1	5	6	10021.60546	-0.00002
6	0	6	5	→	5	0	5	4	10123.11578	0.00054
6	0	6	6	→	5	0	5	5	10123.13243	0.00161
6	0	6	7	→	5	0	5	6	10123.15193	-0.00228
6	1	6	5	→	5	0	5	4	10165.53159	-0.00050
6	1	6	6	→	5	0	5	5	10165.56215	0.00006
6	1	6	7	→	5	0	5	6	10165.57205	-0.00111
6	2	5	6	→	5	2	4	5	11339.43647	-0.00007
6	2	5	5	→	5	2	4	4	11339.58280	0.00216
6	2	5	7	→	5	2	4	6	11339.58280	-0.00030
7	0	7	7	→	6	1	6	6	11614.27710	0.00052
7	0	7	6	→	6	1	6	5	11614.28749	0.00067
7	0	7	8	→	6	1	6	7	11614.31245	0.00025

7	1	7	7	→	6	1	6	6	11631.15848	-0.00082
7	1	7	6	→	6	1	6	5	11631.16611	0.00147
7	1	7	8	→	6	1	6	7	11631.19058	-0.00007
7	0	7	6	→	6	0	6	5	11656.70311	-0.00056
7	0	7	7	→	6	0	6	6	11656.70868	0.00084
7	0	7	8	→	6	0	6	7	11656.73011	-0.00104
7	1	7	6	→	6	0	6	5	11673.58117	-0.00032
7	1	7	7	→	6	0	6	6	11673.59153	0.00096
7	1	7	8	→	6	0	6	7	11673.60946	-0.00015
6	2	5	5	→	5	1	4	4	12705.53239	0.00016
6	2	5	7	→	5	1	4	6	12705.59728	-0.00100
6	2	5	6	→	5	1	4	5	12705.76421	0.00028
6	2	4	6	→	5	2	3	5	12909.05692	-0.00015
6	2	4	5	→	5	2	3	4	12909.17398	-0.00110
6	2	4	7	→	5	2	3	6	12909.18557	0.00108
7	2	6	7	→	6	2	5	6	13030.95222	-0.00030
7	2	6	6	→	6	2	5	5	13031.03270	0.00126
7	2	6	8	→	6	2	5	7	13031.04039	-0.00103
8	0	8	8	→	7	1	7	7	13183.11388	-0.00139
8	0	8	7	→	7	1	7	6	13183.12163	0.00146
8	0	8	9	→	7	1	7	8	13183.14060	0.00029
8	0	8	7	→	7	0	7	6	13199.99826	0.00026
8	0	8	8	→	7	0	7	7	13199.99826	0.00026
8	0	8	9	→	7	0	7	8	13200.01772	-0.00104

Table V(D). Microwave transitions of the $^{13}C_3$ isotopologue of 23DFBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	1	4	4	→	3	1	3	3	6845.91552	-0.00028
4	1	4	3	→	3	1	3	2	6846.00380	-0.00058
4	1	4	5	→	3	1	3	4	6846.05863	-0.00005
4	0	4	3	→	3	0	3	2	7072.09462	-0.00031
4	0	4	4	→	3	0	3	3	7072.20024	-0.00121
4	0	4	5	→	3	0	3	4	7072.20773	0.00131
4	1	4	3	→	3	0	3	2	7304.90536	0.00046
4	1	4	5	→	3	0	3	4	7305.04026	-0.00006
4	2	3	4	→	3	2	2	3	7730.94280	-0.00021
4	2	3	5	→	3	2	2	4	7731.46096	0.00038
4	2	3	3	→	3	2	2	2	7731.59258	-0.00095
5	0	5	5	→	4	1	4	4	8349.92697	0.00002
5	0	5	4	→	4	1	4	3	8349.99913	-0.00021
5	0	5	6	→	4	1	4	5	8350.03793	0.00101
4	1	3	4	→	3	1	2	3	8378.84369	0.00076
4	1	3	3	→	3	1	2	2	8378.91109	-0.00045
4	1	3	5	→	3	1	2	4	8378.96688	0.00071
5	1	5	5	→	4	1	4	4	8455.54344	-0.00037
5	1	5	4	→	4	1	4	3	8455.57437	0.00045
5	1	5	6	→	4	1	4	5	8455.61891	0.00023
5	0	5	4	→	4	0	4	3	8582.80885	-0.00047
5	0	5	5	→	4	0	4	4	8582.85409	0.00038
5	0	5	6	→	4	0	4	5	8582.87066	-0.00017
5	1	5	4	→	4	0	4	3	8688.38316	-0.00073
5	1	5	6	→	4	0	4	5	8688.45259	0.00000
5	1	5	5	→	4	0	4	4	8688.46974	-0.00083
6	0	6	6	→	5	1	5	5	9991.73237	0.00103
6	0	6	5	→	5	1	5	4	9991.75474	-0.00305
6	0	6	7	→	5	1	5	6	9991.78933	-0.00036
6	0	6	5	→	5	0	5	4	10097.33368	0.00131
6	0	6	6	→	5	0	5	5	10097.34980	0.00160
6	0	6	7	→	5	0	5	6	10097.37121	-0.00024
6	1	6	5	→	5	0	5	4	10141.83620	0.00067
6	1	6	6	→	5	0	5	5	10141.86585	-0.00033
6	1	6	7	→	5	0	5	6	10141.87806	0.00129
5	2	3	5	→	4	2	2	4	10709.31885	-0.00099
5	2	3	6	→	4	2	2	5	10709.58175	0.00084
5	2	3	4	→	4	2	2	3	10709.60008	-0.00079
6	2	5	6	→	5	2	4	5	11302.14871	0.00057
6	2	5	5	→	5	2	4	4	11302.29518	0.00234
6	2	5	7	→	5	2	4	6	11302.29518	-0.00004
7	0	7	7	→	6	1	6	6	11581.84985	-0.00053

7	0	7	6	→	6	1	6	5	11581.86073	-0.00015
7	0	7	8	→	6	1	6	7	11581.88622	-0.00005
7	1	7	6	→	6	0	6	5	11644.23048	-0.00081
7	1	7	7	→	6	0	6	6	11644.24143	0.00072
7	1	7	8	→	6	0	6	7	11644.25930	-0.00020
7	1	6	7	→	6	2	5	6	12550.30064	0.00027
7	1	6	8	→	6	2	5	7	12550.47534	0.00025
7	1	6	6	→	6	2	5	5	12550.47534	-0.00215
6	2	5	5	→	5	1	4	4	12700.08007	-0.00059
6	2	5	7	→	5	1	4	6	12700.14674	-0.00009
6	2	5	6	→	5	1	4	5	12700.31295	0.00006
6	2	4	6	→	5	2	3	5	12854.40045	0.00047
6	2	4	5	→	5	2	3	4	12854.51855	-0.00107
6	2	4	7	→	5	2	3	6	12854.52979	0.00109
7	2	6	7	→	6	2	5	6	12990.90161	-0.00006
7	2	6	6	→	6	2	5	5	12990.98215	0.00101
7	2	6	8	→	6	2	5	7	12990.99008	-0.00099
8	0	8	8	→	7	1	7	7	13147.36021	-0.00087
8	0	8	7	→	7	1	7	6	13147.36779	0.00171
8	0	8	9	→	7	1	7	8	13147.38693	0.00069
8	1	8	8	→	7	1	7	7	13154.29397	0.00105
8	1	8	7	→	7	1	7	6	13154.29397	-0.00224
8	1	8	9	→	7	1	7	8	13154.31673	0.00017
8	0	8	7	→	7	0	7	6	13165.23313	-0.00021
8	0	8	8	→	7	0	7	7	13165.23313	-0.00029
8	0	8	9	→	7	0	7	8	13165.25303	-0.00112
8	1	8	7	→	7	0	7	6	13172.16505	0.00159
8	1	8	8	→	7	0	7	7	13172.16505	-0.00022
8	1	8	9	→	7	0	7	8	13172.18420	-0.00027

Table V(E). Microwave transitions of the $^{13}C_4$ isotopologue of 23DFBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	1	4	4	→	3	1	3	3	6821.81601	0.00033
4	1	4	3	→	3	1	3	2	6821.90374	-0.00069
4	1	4	5	→	3	1	3	4	6821.95924	0.00050
4	0	4	3	→	3	0	3	2	7045.73405	-0.00108
4	0	4	4	→	3	0	3	3	7045.84774	0.00279
4	0	4	5	→	3	0	3	4	7045.84774	0.00011
4	1	4	3	→	3	0	3	2	7274.35526	-0.00056
4	1	4	5	→	3	0	3	4	7274.49286	0.00022
4	1	4	4	→	3	0	3	3	7274.58481	0.00047
4	2	3	4	→	3	2	2	3	7706.29209	0.00095
4	2	3	5	→	3	2	2	4	7706.81378	0.00140
4	2	3	3	→	3	2	2	2	7706.94727	0.00100
5	0	5	5	→	4	1	4	4	8321.93405	-0.00043
5	0	5	4	→	4	1	4	3	8322.00571	-0.00136
5	0	5	6	→	4	1	4	5	8322.04536	0.00071
4	1	3	4	→	3	1	2	3	8352.31366	0.00020
4	1	3	3	→	3	1	2	2	8352.37980	-0.00006
4	1	3	5	→	3	1	2	4	8352.43621	0.00026
5	1	5	5	→	4	1	4	4	8425.22738	-0.00036
5	1	5	4	→	4	1	4	3	8425.25793	0.00047
5	1	5	6	→	4	1	4	5	8425.30234	0.00002
5	0	5	4	→	4	0	4	3	8550.62802	0.00026
5	0	5	5	→	4	0	4	4	8550.67390	0.00004
5	0	5	6	→	4	0	4	5	8550.68962	-0.00004
5	1	5	4	→	4	0	4	3	8653.87830	0.00015
5	1	5	6	→	4	0	4	5	8653.94798	0.00064
5	1	5	5	→	4	0	4	4	8653.96662	-0.00051
6	0	6	6	→	5	1	5	5	9956.47732	0.00047
6	0	6	5	→	5	1	5	4	9956.50038	-0.00262
6	0	6	7	→	5	1	5	6	9956.53518	0.00023
6	0	6	5	→	5	0	5	4	10059.75479	0.00140
6	0	6	6	→	5	0	5	5	10059.77132	0.00121
6	0	6	7	→	5	0	5	6	10059.78910	-0.00353
6	1	6	5	→	5	0	5	4	10103.09998	-0.00095
6	1	6	6	→	5	0	5	5	10103.13178	-0.00086
6	1	6	7	→	5	0	5	6	10103.14342	0.00107
5	2	3	5	→	4	2	2	4	10679.56274	0.00026
5	2	3	6	→	4	2	2	5	10679.82610	0.00011
5	2	3	4	→	4	2	2	3	10679.84231	-0.00348
6	2	5	6	→	5	2	4	5	11263.84321	-0.00121
6	2	5	5	→	5	2	4	4	11263.99169	0.00265
6	2	5	7	→	5	2	4	6	11263.99169	0.00010

7	0	7	7	→	6	1	6	6	11540.02831	0.00014
7	0	7	6	→	6	1	6	5	11540.03971	0.00141
7	0	7	8	→	6	1	6	7	11540.06418	0.00043
7	1	7	7	→	6	1	6	6	11557.36627	-0.00085
7	1	7	6	→	6	1	6	5	11557.37339	0.00127
7	1	7	8	→	6	1	6	7	11557.39751	-0.00071
7	0	7	6	→	6	0	6	5	11583.38482	-0.00102
7	0	7	7	→	6	0	6	6	11583.39219	0.00149
7	0	7	8	→	6	0	6	7	11583.41305	-0.00042
7	1	7	6	→	6	0	6	5	11600.72007	0.00041
7	1	7	7	→	6	0	6	6	11600.72983	0.00018
7	1	7	8	→	6	0	6	7	11600.74804	0.00009
7	1	6	7	→	6	2	5	6	12515.35129	0.00079
7	1	6	8	→	6	2	5	7	12515.52692	0.00093
7	1	6	6	→	6	2	5	5	12515.52692	-0.00145
6	2	5	5	→	5	1	4	4	12640.76638	-0.00029
6	2	5	7	→	5	1	4	6	12640.83450	0.00034
6	2	5	6	→	5	1	4	5	12641.00558	-0.00028
6	2	4	6	→	5	2	3	5	12816.29237	0.00044
6	2	4	5	→	5	2	3	4	12816.41067	-0.00068
6	2	4	7	→	5	2	3	6	12816.42266	0.00175
7	2	6	7	→	6	2	5	6	12945.62777	-0.00050
7	2	6	6	→	6	2	5	5	12945.70778	0.00065
7	2	6	8	→	6	2	5	7	12945.71607	-0.00117
8	0	8	8	→	7	1	7	7	13099.41068	-0.00099
8	0	8	7	→	7	1	7	6	13099.41737	0.00102
8	0	8	9	→	7	1	7	8	13099.43653	-0.00001
8	1	8	8	→	7	1	7	7	13106.11031	0.00034
8	1	8	7	→	7	1	7	6	13106.11031	-0.00262
8	1	8	9	→	7	1	7	8	13106.13317	-0.00015
8	0	8	7	→	7	0	7	6	13116.74980	-0.00037
8	0	8	8	→	7	0	7	7	13116.74980	-0.00082
8	0	8	9	→	7	0	7	8	13116.77130	0.00028
8	1	8	7	→	7	0	7	6	13123.44939	0.00265
8	1	8	8	→	7	0	7	7	13123.44939	0.00047
8	1	8	9	→	7	0	7	8	13123.46774	-0.00005

Table V(F). Microwave transitions of the $^{13}C_5$ isotopologue of 23DFBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	1	4	4	→	3	1	3	3	6823.19980	0.00004
4	1	4	3	→	3	1	3	2	6823.28783	0.00018
4	1	4	5	→	3	1	3	4	6823.34229	0.00007
4	0	4	3	→	3	0	3	2	7036.30502	0.00047
4	0	4	4	→	3	0	3	3	7036.41558	0.00177
4	0	4	5	→	3	0	3	4	7036.41558	-0.00094
4	1	4	3	→	3	0	3	2	7241.26834	0.00016
4	1	4	5	→	3	0	3	4	7241.40336	0.00009
4	1	4	4	→	3	0	3	3	7241.48922	-0.00102
4	2	3	4	→	3	2	2	3	7726.87957	-0.00013
4	2	3	5	→	3	2	2	4	7727.40112	0.00008
4	2	3	3	→	3	2	2	2	7727.53340	-0.00156
5	0	5	5	→	4	1	4	4	8333.05705	0.00023
5	0	5	4	→	4	1	4	3	8333.12465	-0.00092
5	0	5	6	→	4	1	4	5	8333.16441	0.00058
4	1	3	4	→	3	1	2	3	8375.51378	-0.00043
4	1	3	3	→	3	1	2	2	8375.57614	-0.00010
4	1	3	5	→	3	1	2	4	8375.63308	-0.00019
5	1	5	5	→	4	1	4	4	8422.87316	-0.00062
5	1	5	4	→	4	1	4	3	8422.90366	0.00065
5	1	5	6	→	4	1	4	5	8422.94820	0.00022
5	0	5	4	→	4	0	4	3	8538.08934	0.00013
5	0	5	5	→	4	0	4	4	8538.13391	0.00065
5	0	5	6	→	4	0	4	5	8538.14987	-0.00070
5	1	5	4	→	4	0	4	3	8627.86634	-0.00030
5	1	5	6	→	4	0	4	5	8627.93484	0.00012
5	1	5	5	→	4	0	4	4	8627.95089	0.00067
6	0	6	6	→	5	1	5	5	9957.36579	0.00054
6	0	6	5	→	5	1	5	4	9957.38664	-0.00308
6	0	6	7	→	5	1	5	6	9957.42186	-0.00006
6	0	6	5	→	5	0	5	4	10047.16766	0.00051
6	0	6	6	→	5	0	5	5	10047.18263	0.00042
6	0	6	7	→	5	0	5	6	10047.20574	-0.00033
6	1	6	5	→	5	0	5	4	10083.73783	-0.00011
6	1	6	6	→	5	0	5	5	10083.76507	-0.00134
6	1	6	7	→	5	0	5	6	10083.78036	0.00154
5	2	3	5	→	4	2	2	4	10740.12588	-0.00069
5	2	3	6	→	4	2	2	5	10740.38673	-0.00022
5	2	3	4	→	4	2	2	3	10740.40873	0.00300
6	2	5	6	→	5	2	4	5	11276.79726	0.00008
6	2	5	5	→	5	2	4	4	11276.94241	0.00192
6	2	5	7	→	5	2	4	6	11276.94241	-0.00079

7	0	7	7	→	6	1	6	6	11534.41276	-0.00037
7	0	7	6	→	6	1	6	5	11534.42393	0.00121
7	0	7	8	→	6	1	6	7	11534.44858	0.00035
7	1	7	7	→	6	1	6	6	11548.61101	-0.00093
7	1	7	6	→	6	1	6	5	11548.61800	0.00092
7	1	7	8	→	6	1	6	7	11548.64323	0.00006
7	0	7	6	→	6	0	6	5	11570.99345	-0.00006
7	0	7	7	→	6	0	6	6	11570.99866	0.00134
7	0	7	8	→	6	0	6	7	11571.02045	-0.00053
7	1	7	6	→	6	0	6	5	11585.18668	-0.00119
7	1	7	7	→	6	0	6	6	11585.19728	0.00114
7	1	7	8	→	6	0	6	7	11585.21590	-0.00001
6	2	5	5	→	5	1	4	4	12538.75934	-0.00022
6	2	5	7	→	5	1	4	6	12538.82576	-0.00001
6	2	5	6	→	5	1	4	5	12538.99207	0.00051
7	1	6	7	→	6	2	5	6	12581.46418	0.00068
7	1	6	8	→	6	2	5	7	12581.63149	0.00048
7	1	6	6	→	6	2	5	5	12581.63149	-0.00080
6	2	4	6	→	5	2	3	5	12870.57018	-0.00041
6	2	4	5	→	5	2	3	4	12870.68447	-0.00005
6	2	4	7	→	5	2	3	6	12870.69430	-0.00082
7	2	6	7	→	6	2	5	6	12951.25634	-0.00039
7	2	6	6	→	6	2	5	5	12951.33498	0.00041
7	2	6	8	→	6	2	5	7	12951.34421	-0.00056
8	1	8	8	→	7	1	7	7	13095.12864	0.00090
8	1	8	7	→	7	1	7	6	13095.12864	-0.00229
8	1	8	9	→	7	1	7	8	13095.15036	-0.00093
8	0	8	7	→	7	0	7	6	13104.00137	-0.00027
8	0	8	8	→	7	0	7	7	13104.00137	0.00002
8	0	8	9	→	7	0	7	8	13104.02302	0.00070
8	1	8	7	→	7	0	7	6	13109.32640	0.00111
8	1	8	8	→	7	0	7	7	13109.32640	-0.00016
8	1	8	9	→	7	0	7	8	13109.34604	-0.00019

Table V(G). Microwave transitions of the $^{13}C_6$ isotopologue of 23DFBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	1	4	4	→	3	1	3	3	6839.16840	-0.00007
4	1	4	3	→	3	1	3	2	6839.25595	-0.00010
4	1	4	5	→	3	1	3	4	6839.31117	0.00074
4	0	4	3	→	3	0	3	2	7055.76535	-0.00072
4	0	4	4	→	3	0	3	3	7055.87010	-0.00111
4	0	4	5	→	3	0	3	4	7055.87818	0.00156
4	1	4	3	→	3	0	3	2	7267.51811	-0.00152
4	1	4	5	→	3	0	3	4	7267.65319	0.00025
4	1	4	4	→	3	0	3	3	7267.73651	0.00067
4	2	3	4	→	3	2	2	3	7739.73293	0.00063
4	2	3	5	→	3	2	2	4	7740.24826	0.00038
4	2	3	3	→	3	2	2	2	7740.37968	-0.00065
5	0	5	5	→	4	1	4	4	8350.12456	-0.00025
5	0	5	4	→	4	1	4	3	8350.19272	-0.00095
5	0	5	6	→	4	1	4	5	8350.23208	0.00035
4	1	3	4	→	3	1	2	3	8389.28027	-0.00025
4	1	3	3	→	3	1	2	2	8389.34664	0.00089
4	1	3	5	→	3	1	2	4	8389.40106	0.00034
5	1	5	5	→	4	1	4	4	8443.70084	-0.00043
5	1	5	4	→	4	1	4	3	8443.73090	-0.00006
5	1	5	6	→	4	1	4	5	8443.77616	0.00048
5	0	5	4	→	4	0	4	3	8561.94614	-0.00109
5	0	5	5	→	4	0	4	4	8561.99064	0.00120
5	0	5	6	→	4	0	4	5	8562.00787	-0.00019
5	1	5	4	→	4	0	4	3	8655.48426	-0.00026
5	1	5	6	→	4	0	4	5	8655.55253	0.00053
5	1	5	5	→	4	0	4	4	8655.56635	0.00045
6	0	6	6	→	5	1	5	5	9981.06868	0.00031
6	0	6	5	→	5	1	5	4	9981.09124	-0.00211
6	0	6	7	→	5	1	5	6	9981.12578	0.00041
6	0	6	5	→	5	0	5	4	10074.63193	0.00129
6	0	6	6	→	5	0	5	5	10074.64590	0.00107
6	0	6	7	→	5	0	5	6	10074.66752	-0.00180
6	1	6	5	→	5	0	5	4	10113.05059	-0.00075
6	1	6	6	→	5	0	5	5	10113.07753	-0.00137
6	1	6	7	→	5	0	5	6	10113.09372	0.00176
5	2	3	5	→	4	2	2	4	10749.27726	0.00015
5	2	3	6	→	4	2	2	5	10749.53355	-0.00085
5	2	3	4	→	4	2	2	3	10749.55298	-0.00051
6	2	5	6	→	5	2	4	5	11300.31039	-0.00013
6	2	5	5	→	5	2	4	4	11300.45519	0.00143
6	2	5	7	→	5	2	4	6	11300.45519	-0.00106

7	0	7	7	→	6	1	6	6	11563.62294	0.00033
7	0	7	6	→	6	1	6	5	11563.63270	0.00003
7	0	7	8	→	6	1	6	7	11563.65834	0.00028
7	1	7	7	→	6	1	6	6	11578.66196	-0.00062
7	1	7	6	→	6	1	6	5	11578.66932	0.00114
7	1	7	8	→	6	1	6	7	11578.69390	-0.00023
7	0	7	6	→	6	0	6	5	11602.05723	0.00386
7	0	7	7	→	6	0	6	6	11602.05723	0.00055
7	0	7	8	→	6	0	6	7	11602.08015	-0.00055
7	1	7	6	→	6	0	6	5	11617.08723	-0.00164
7	1	7	7	→	6	0	6	6	11617.09743	0.00077
7	1	7	8	→	6	0	6	7	11617.11721	0.00043
7	1	6	7	→	6	2	5	6	12594.23725	0.00009
7	1	6	8	→	6	2	5	7	12594.40479	0.00036
7	1	6	6	→	6	2	5	5	12594.40479	-0.00108
6	2	5	5	→	5	1	4	4	12596.26442	-0.00015
6	2	5	7	→	5	1	4	6	12596.32936	0.00013
6	2	5	6	→	5	1	4	5	12596.48838	-0.00039
6	2	4	6	→	5	2	3	5	12886.69227	0.00003
6	2	4	5	→	5	2	3	4	12886.80739	0.00036
6	2	4	7	→	5	2	3	6	12886.81707	0.00026
7	2	6	7	→	6	2	5	6	12980.80860	-0.00040
7	2	6	6	→	6	2	5	5	12980.88859	0.00107
7	2	6	8	→	6	2	5	7	12980.89707	-0.00038
8	0	8	8	→	7	1	7	7	13123.79435	-0.00058
8	0	8	7	→	7	1	7	6	13123.80084	0.00090
8	0	8	9	→	7	1	7	8	13123.81832	-0.00174
8	1	8	8	→	7	1	7	7	13129.48387	0.00199
8	1	8	7	→	7	1	7	6	13129.48387	-0.00155
8	1	8	9	→	7	1	7	8	13129.50563	-0.00007
8	0	8	8	→	7	0	7	7	13138.83565	0.00074
8	0	8	7	→	7	0	7	6	13138.83565	0.00021
8	0	8	9	→	7	0	7	8	13138.85603	-0.00010
8	1	8	7	→	7	0	7	6	13144.52141	0.00049
8	1	8	8	→	7	0	7	7	13144.52141	-0.00045
8	1	8	9	→	7	0	7	8	13144.54180	0.00002

Table V(H). Microwave transitions of the $^{13}C_7$ isotopologue of 23DFBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	1	4	4	→	3	1	3	3	6810.34709	0.00034
4	1	4	3	→	3	1	3	2	6810.43568	-0.00024
4	1	4	5	→	3	1	3	4	6810.49031	0.00000
4	0	4	3	→	3	0	3	2	7039.33363	0.00013
4	0	4	4	→	3	0	3	3	7039.43973	-0.00083
4	0	4	5	→	3	0	3	4	7039.44666	0.00107
4	1	4	3	→	3	0	3	2	7280.33874	0.00060
4	1	4	5	→	3	0	3	4	7280.47545	0.00077
4	1	4	4	→	3	0	3	3	7280.56427	-0.00026
4	2	3	4	→	3	2	2	3	7683.76386	-0.00009
4	2	3	5	→	3	2	2	4	7684.28294	-0.00030
4	2	3	3	→	3	2	2	2	7684.41619	-0.00044
5	0	5	5	→	4	1	4	4	8302.55255	0.00003
5	0	5	4	→	4	1	4	3	8302.62536	-0.00122
5	0	5	6	→	4	1	4	5	8302.66465	0.00061
4	1	3	4	→	3	1	2	3	8327.13616	0.00000
4	1	3	3	→	3	1	2	2	8327.20736	0.00093
4	1	3	5	→	3	1	2	4	8327.26049	-0.00046
5	1	5	5	→	4	1	4	4	8413.11614	0.00018
5	1	5	4	→	4	1	4	3	8413.14688	0.00054
5	1	5	6	→	4	1	4	5	8413.19146	0.00024
5	0	5	4	→	4	0	4	3	8543.63105	-0.00018
5	0	5	5	→	4	0	4	4	8543.67704	0.00055
5	0	5	6	→	4	0	4	5	8543.69268	-0.00045
5	1	5	4	→	4	0	4	3	8654.15077	-0.00022
5	1	5	6	→	4	0	4	5	8654.22060	0.00029
5	1	5	5	→	4	0	4	4	8654.23986	-0.00007
6	0	6	6	→	5	1	5	5	9939.94603	0.00057
6	0	6	5	→	5	1	5	4	9939.96966	-0.00299
6	0	6	7	→	5	1	5	6	9940.00510	0.00055
6	0	6	6	→	5	0	5	5	10050.50943	0.00053
6	0	6	7	→	5	0	5	6	10050.52903	-0.00270
6	1	6	5	→	5	0	5	4	10097.59685	-0.00048
6	1	6	6	→	5	0	5	5	10097.62888	-0.00043
6	1	6	7	→	5	0	5	6	10097.64034	0.00142
5	2	3	5	→	4	2	2	4	10631.91324	-0.00109
5	2	3	6	→	4	2	2	5	10632.17847	0.00113
6	2	5	6	→	5	2	4	5	11239.32156	0.00037
6	2	5	5	→	5	2	4	4	11239.46819	0.00137
6	2	5	7	→	5	2	4	6	11239.46819	-0.00097
7	0	7	7	→	6	1	6	6	11524.51446	0.00034
7	0	7	6	→	6	1	6	5	11524.52600	0.00113

7	0	7	8	→	6	1	6	7	11524.55032	-0.00001
7	1	7	7	→	6	1	6	6	11543.63844	-0.00018
7	1	7	6	→	6	1	6	5	11543.64508	0.00108
7	1	7	8	→	6	1	6	7	11543.66976	-0.00038
7	0	7	6	→	6	0	6	5	11571.62875	-0.00105
7	0	7	7	→	6	0	6	6	11571.63658	0.00205
7	0	7	8	→	6	0	6	7	11571.65705	-0.00046
7	1	7	6	→	6	0	6	5	11590.74879	-0.00014
7	1	7	7	→	6	0	6	6	11590.75924	0.00020
7	1	7	8	→	6	0	6	7	11590.77766	0.00033
7	1	6	7	→	6	2	5	6	12459.07353	-0.00035
7	1	6	8	→	6	2	5	7	12459.25313	0.00101
7	1	6	6	→	6	2	5	5	12459.25313	-0.00180
6	2	5	5	→	5	1	4	4	12674.54042	-0.00068
6	2	5	7	→	5	1	4	6	12674.60772	-0.00022
6	2	5	6	→	5	1	4	5	12674.77662	0.00002
6	2	4	6	→	5	2	3	5	12767.90970	0.00057
6	2	4	5	→	5	2	3	4	12768.02960	-0.00140
6	2	4	7	→	5	2	3	6	12768.04063	0.00083
7	2	6	7	→	6	2	5	6	12922.08738	0.00010
7	2	6	6	→	6	2	5	5	12922.16855	0.00117
7	2	6	8	→	6	2	5	7	12922.17716	-0.00014
8	0	8	8	→	7	1	7	7	13083.61772	-0.00107
8	0	8	7	→	7	1	7	6	13083.62478	0.00094
8	0	8	9	→	7	1	7	8	13083.64427	0.00021
8	1	8	8	→	7	1	7	7	13091.11896	0.00198
8	1	8	7	→	7	1	7	6	13091.11896	-0.00123
8	1	8	9	→	7	1	7	8	13091.14003	-0.00060
8	0	8	7	→	7	0	7	6	13102.74305	0.00008
8	0	8	8	→	7	0	7	7	13102.74305	-0.00024
8	0	8	9	→	7	0	7	8	13102.76387	-0.00001
8	1	8	7	→	7	0	7	6	13110.24039	0.00107
8	1	8	8	→	7	0	7	7	13110.24039	-0.00110
8	1	8	9	→	7	0	7	8	13110.25988	-0.00057

Table V(I). Microwave transitions of the ^{15}N isotopologue of 23DFBN in MHz

J'	K_a'	K_c'	→	J"	K_a"	K_c"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	0	4	→	3	1	3	6483.30002	-0.00005
4	1	4	→	3	1	3	6739.78844	-0.00051
4	0	4	→	3	0	3	6973.61163	-0.00030
4	1	4	→	3	0	3	7230.10107	0.00026
4	2	3	→	3	2	2	7591.69042	-0.00012
5	0	5	→	4	1	4	8208.58252	-0.00020
4	1	3	→	3	1	2	8225.69343	-0.00009
4	2	2	→	3	2	1	8275.90562	0.00017
5	1	5	→	4	1	4	8328.62521	-0.00012
5	0	5	→	4	0	4	8465.07183	0.00023
5	1	5	→	4	0	4	8585.11360	-0.00061
5	2	4	→	4	2	3	9384.14825	-0.00024
6	0	6	→	5	1	5	9836.71398	0.00045
6	1	6	→	5	1	5	9888.91919	0.00029
6	0	6	→	5	0	5	9956.75658	0.00045
6	1	6	→	5	0	5	10008.96154	0.00003
5	1	4	→	4	1	3	10045.24740	0.00008
5	2	3	→	4	2	2	10481.96415	0.00024
6	2	5	→	5	2	4	11115.16658	-0.00003
7	0	7	→	6	1	6	11410.00230	0.00083
7	1	7	→	6	1	6	11431.61657	-0.00021
7	0	7	→	6	0	6	11462.20684	-0.00001
7	1	7	→	6	0	6	11483.82208	-0.00008
6	1	5	→	5	1	4	11694.37221	-0.00005
7	1	6	→	6	2	5	12279.41112	-0.00007
6	2	4	→	5	2	3	12598.97933	-0.00013
6	2	5	→	5	1	4	12619.04761	-0.00020
7	2	6	→	6	2	5	12785.45216	0.00000
8	0	8	→	7	1	7	12956.24197	0.00012
8	1	8	→	7	1	7	12964.88516	-0.00083
8	0	8	→	7	0	7	12977.85752	0.00036
8	1	8	→	7	0	7	12986.50107	-0.00023
7	1	6	→	6	1	5	13204.08728	0.00054
7	2	6	→	6	1	5	13710.12776	0.00005
8	1	7	→	7	2	6	14151.04010	-0.00023

Appendix VI. Microwave transitions of the 2,4-difluorobenzonitrile (24DFBN) and its isotopologues

Table VI(A). Microwave transitions of the parent 24DFBN in MHz

J'	$K_{a'}$	$K_{c'}$	F'	→	J"	$K_{a"}$	$K_{c"}$	F"	ν_{obs}	$\nu_{obs.-calc.}$
4	1	4	4	→	3	1	3	3	6079.10150	0.00012
4	1	4	3	→	3	1	3	2	6079.21147	0.00016
4	1	4	5	→	3	1	3	4	6079.26165	0.00006
4	0	4	3	→	3	0	3	2	6389.74341	0.00019
4	0	4	4	→	3	0	3	3	6389.85815	-0.00172
4	0	4	5	→	3	0	3	4	6389.86929	0.00102
4	2	3	4	→	3	2	2	3	6548.75652	-0.00027
4	2	3	5	→	3	2	2	4	6549.32666	0.00043
4	2	3	3	→	3	2	2	2	6549.47197	-0.00047
4	3	2	4	→	3	3	1	3	6595.65196	-0.00001
4	3	2	5	→	3	3	1	4	6596.90616	0.00066
4	3	2	3	→	3	3	1	2	6597.38959	-0.00066
4	3	1	4	→	3	3	0	3	6601.03336	-0.00013
4	3	1	5	→	3	3	0	4	6602.29042	0.00161
4	3	1	3	→	3	3	0	2	6602.77366	-0.00032
5	0	5	5	→	4	1	4	4	6670.50706	0.00019
5	0	5	4	→	4	1	4	3	6670.72490	0.00126
5	0	5	6	→	4	1	4	5	6670.73744	-0.00049
4	2	2	4	→	3	2	1	3	6722.04968	0.00040
4	2	2	5	→	3	2	1	4	6722.64219	0.00001
4	2	2	3	→	3	2	1	2	6722.79176	0.00018
4	1	3	4	→	3	1	2	3	6974.84870	-0.00012
4	1	3	3	→	3	1	2	2	6974.94850	0.00004
4	1	3	5	→	3	1	2	4	6975.00997	-0.00009
5	1	5	5	→	4	1	4	4	7570.91437	0.00012
5	1	5	4	→	4	1	4	3	7570.95439	0.00014
5	1	5	6	→	4	1	4	5	7570.99822	-0.00010
5	0	5	4	→	4	0	4	3	7874.32376	0.00018
5	0	5	6	→	4	0	4	5	7874.39876	0.00089
5	0	5	5	→	4	0	4	4	7874.39876	-0.00192
5	2	4	5	→	4	2	3	4	8163.82687	0.00017
5	2	4	6	→	4	2	3	5	8164.12153	0.00004
5	2	4	4	→	4	2	3	3	8164.15132	0.00014
5	3	3	5	→	4	3	2	4	8256.40336	-0.00003
5	3	3	6	→	4	3	2	5	8257.05363	0.00013
5	3	3	4	→	4	3	2	3	8257.21210	-0.00006
5	3	2	5	→	4	3	1	4	8275.07388	-0.00036
5	3	2	6	→	4	3	1	5	8275.72808	-0.00021
5	3	2	4	→	4	3	1	3	8275.88704	-0.00057

6	0	6	6	→	5	1	5	5	8411.57397	-0.00077
6	0	6	5	→	5	1	5	4	8411.69724	0.00103
6	0	6	7	→	5	1	5	6	8411.71450	-0.00060
5	2	3	5	→	4	2	2	4	8493.11302	0.00017
5	2	3	6	→	4	2	2	5	8493.43191	-0.00036
5	2	3	4	→	4	2	2	3	8493.46346	-0.00042
5	1	4	5	→	4	1	3	4	8678.65137	-0.00059
5	1	4	4	→	4	1	3	3	8678.68320	0.00034
5	1	4	6	→	4	1	3	5	8678.73354	-0.00052
5	1	5	4	→	4	0	4	3	8774.55375	-0.00044
5	1	5	6	→	4	0	4	5	8774.65853	0.00027
5	1	5	5	→	4	0	4	4	8774.80756	-0.00050
6	1	6	6	→	5	1	5	5	9048.19962	0.00062
6	1	6	5	→	5	1	5	4	9048.21322	-0.00020
6	1	6	7	→	5	1	5	6	9048.24810	0.00009
6	0	6	5	→	5	0	5	4	9311.92744	0.00063
6	0	6	7	→	5	0	5	6	9311.97432	-0.00116
6	0	6	6	→	5	0	5	5	9311.98279	0.00066
6	2	5	6	→	5	2	4	5	9764.08256	-0.00079
6	2	5	5	→	5	2	4	4	9764.25436	0.00109
6	2	5	7	→	5	2	4	6	9764.25436	-0.00030
6	4	3	6	→	5	4	2	5	9904.99866	0.00024
6	4	3	7	→	5	4	2	6	9905.66477	0.00019
6	4	3	5	→	5	4	2	4	9905.80704	-0.00013
6	4	2	6	→	5	4	1	5	9906.33479	-0.00006
6	4	2	7	→	5	4	1	6	9907.00171	0.00039
6	4	2	5	→	5	4	1	4	9907.14363	-0.00033
6	3	4	6	→	5	3	3	5	9920.10655	-0.00039
6	3	4	7	→	5	3	3	6	9920.48906	-0.00007
6	3	4	5	→	5	3	3	4	9920.54785	-0.00020
6	1	6	5	→	5	0	5	4	9948.44381	-0.00022
6	1	6	7	→	5	0	5	6	9948.50880	0.00041
6	1	6	6	→	5	0	5	5	9948.60637	-0.00001
6	3	3	6	→	5	3	2	5	9969.08585	-0.00074
6	3	3	7	→	5	3	2	6	9969.47593	0.00015
6	3	3	5	→	5	3	2	4	9969.53547	-0.00020
7	0	7	7	→	6	1	6	6	10082.52297	-0.00047
7	0	7	6	→	6	1	6	5	10082.59096	0.00044
7	0	7	8	→	6	1	6	7	10082.60890	-0.00059
6	2	4	6	→	5	2	3	5	10295.54273	-0.00039
6	2	4	5	→	5	2	3	4	10295.73642	-0.00010
6	2	4	7	→	5	2	3	6	10295.73642	-0.00037
6	1	5	6	→	5	1	4	5	10350.89328	-0.00223
6	1	5	5	→	5	1	4	4	10350.90281	0.00369
6	1	5	7	→	5	1	4	6	10350.93967	0.00070
7	1	7	7	→	6	1	6	6	10511.53468	-0.00072

7	1	7	6	→	6	1	6	5	10511.53947	0.00051
7	1	7	8	→	6	1	6	7	10511.56578	-0.00020
7	0	7	6	→	6	0	6	5	10719.10772	-0.00002
7	0	7	8	→	6	0	6	7	10719.14173	-0.00067
7	0	7	7	→	6	0	6	6	10719.14860	0.00090
7	1	7	6	→	6	0	6	5	11148.05714	0.00096
7	1	7	8	→	6	0	6	7	11148.09928	0.00039
7	1	7	7	→	6	0	6	6	11148.15951	-0.00014
7	2	6	7	→	6	2	5	6	11347.12722	-0.00038
7	2	6	6	→	6	2	5	5	11347.22532	0.00053
7	2	6	8	→	6	2	5	7	11347.23472	-0.00014
7	5	3	7	→	6	5	2	6	11549.04671	0.00094
7	5	2	7	→	6	5	1	6	11549.12255	-0.00001
7	5	3	8	→	6	5	2	7	11549.70178	0.00073
7	5	2	8	→	6	5	1	7	11549.77694	-0.00093
7	5	3	6	→	6	5	2	5	11549.82511	0.00129
7	5	2	6	→	6	5	1	5	11549.90058	-0.00005
7	4	4	7	→	6	4	3	6	11573.09206	-0.00049
7	4	4	8	→	6	4	3	7	11573.51755	-0.00047
7	4	4	6	→	6	4	3	5	11573.58384	-0.00037
7	4	3	7	→	6	4	2	6	11577.51204	0.00025
7	4	3	8	→	6	4	2	7	11577.93797	-0.00006
7	4	3	6	→	6	4	2	5	11578.00464	0.00033
7	3	5	7	→	6	3	4	6	11584.11778	-0.00036
7	3	5	8	→	6	3	4	7	11584.36209	-0.00006
7	3	5	6	→	6	3	4	5	11584.38347	-0.00050
8	0	8	8	→	7	1	7	7	11684.32732	0.00050
8	0	8	7	→	7	1	7	6	11684.36200	-0.00035
8	0	8	9	→	7	1	7	8	11684.37870	-0.00093
7	3	4	7	→	6	3	3	6	11691.28452	0.00018
7	3	4	8	→	6	3	3	7	11691.53938	0.00016
7	3	4	6	→	6	3	3	5	11691.56201	-0.00029
8	1	8	7	→	7	1	7	6	11962.47245	0.00040
8	1	8	8	→	7	1	7	7	11962.47245	-0.00093
8	1	8	9	→	7	1	7	8	11962.49361	0.00014
7	1	6	6	→	6	1	5	5	11981.25182	0.00054
7	1	6	7	→	6	1	5	6	11981.26128	-0.00054
7	1	6	8	→	6	1	5	7	11981.28245	-0.00019
7	2	5	7	→	6	2	4	6	12109.12922	-0.00060
7	2	5	6	→	6	2	4	5	12109.24526	0.00124
7	2	5	8	→	6	2	4	7	12109.25349	-0.00062
8	0	8	7	→	7	0	7	6	12113.30967	-0.00112
8	0	8	9	→	7	0	7	8	12113.33733	0.00121
8	0	8	8	→	7	0	7	7	12113.33733	-0.00145
8	1	8	7	→	7	0	7	6	12391.41993	-0.00056
8	1	8	9	→	7	0	7	8	12391.45053	0.00057

8	1	8	8	→	7	0	7	7	12391.48552	0.00019
8	2	7	8	→	7	2	6	7	12910.99478	-0.00001
8	2	7	7	→	7	2	6	6	12911.05237	-0.00065
8	2	7	9	→	7	2	6	8	12911.06466	-0.00046
8	6	3	8	→	7	6	2	7	13193.86002	0.00197
8	6	2	8	→	7	6	1	7	13193.86002	-0.00187
8	6	3	9	→	7	6	2	8	13194.49375	0.00252
8	6	2	9	→	7	6	1	8	13194.49375	-0.00132
8	6	3	7	→	7	6	2	6	13194.59793	0.00186
8	6	2	7	→	7	6	1	6	13194.59793	-0.00198
8	5	4	8	→	7	5	3	7	13214.13240	0.00010
8	5	3	8	→	7	5	2	7	13214.43765	-0.00025
8	5	4	9	→	7	5	3	8	13214.57651	0.00030
8	5	4	7	→	7	5	3	6	13214.64085	-0.00025
8	5	3	9	→	7	5	2	8	13214.88230	0.00043
8	5	3	7	→	7	5	2	6	13214.94624	-0.00053
9	0	9	9	→	8	1	8	8	13228.15336	0.00002
9	0	9	8	→	8	1	8	7	13228.17046	-0.00040
9	0	9	10	→	8	1	8	9	13228.18539	-0.00061
8	3	6	8	→	7	3	5	7	13244.71368	0.00011
8	3	6	9	→	7	3	5	8	13244.87786	-0.00063
8	3	6	7	→	7	3	5	6	13244.88618	0.00124
8	4	5	8	→	7	4	4	7	13247.62205	-0.00063
8	4	5	9	→	7	4	4	8	13247.91160	-0.00028
8	4	5	7	→	7	4	4	6	13247.94411	0.00003
8	4	4	8	→	7	4	3	7	13259.62554	0.00055
8	4	4	9	→	7	4	3	8	13259.91512	-0.00063
8	4	4	7	→	7	4	3	6	13259.94845	0.00032
9	1	9	8	→	8	1	8	7	13403.13025	-0.00067
9	1	9	9	→	8	1	8	8	13403.13643	0.00206
9	1	9	10	→	8	1	8	9	13403.14726	-0.00093
5	2	4	4	→	4	1	3	3	13409.45103	0.00004
5	2	4	6	→	4	1	3	5	13409.60124	-0.00002
5	2	4	5	→	4	1	3	4	13410.00709	0.00048
8	3	5	8	→	7	3	4	7	13449.67601	-0.00014
8	3	5	9	→	7	3	4	8	13449.85537	-0.00062
8	3	5	7	→	7	3	4	6	13449.86549	0.00169
9	0	9	8	→	8	0	8	7	13506.28120	0.00065
9	0	9	9	→	8	0	8	8	13506.29952	-0.00037
9	0	9	10	→	8	0	8	9	13506.29952	-0.00032
8	1	7	7	→	7	1	6	6	13559.43330	-0.00034
8	1	7	8	→	7	1	6	7	13559.45073	-0.00215
8	1	7	9	→	7	1	6	8	13559.45964	0.00078
9	1	9	10	→	8	0	8	9	13681.26243	0.00040
9	1	9	9	→	8	0	8	8	13681.27926	-0.00167
8	2	6	8	→	7	2	5	7	13912.00913	0.00011

8	2	6	7	→	7	2	5	6	13912.07795	0.00061
8	2	6	9	→	7	2	5	8	13912.08951	-0.00072
10	1	9	10	→	9	2	8	9	14300.83631	0.00003
10	1	9	11	→	9	2	8	10	14300.98397	-0.00001
10	1	9	9	→	9	2	8	8	14300.98397	-0.00061
9	2	8	9	→	8	2	7	8	14454.39161	0.00010
9	2	8	8	→	8	2	7	7	14454.42821	0.00110
9	2	8	10	→	8	2	7	9	14454.43824	-0.00076
6	2	5	5	→	5	1	4	4	14495.02087	-0.00053
6	2	5	7	→	5	1	4	6	14495.12141	-0.00045
6	2	5	6	→	5	1	4	5	14495.43802	0.00002
10	0	10	10	→	9	1	9	9	14728.26302	-0.00025
10	0	10	9	→	9	1	9	8	14728.27308	0.00227
10	0	10	11	→	9	1	9	10	14728.28308	-0.00079
10	1	10	9	→	9	1	9	8	14835.79131	-0.00135
10	1	10	10	→	9	1	9	9	14835.79842	0.00156
10	1	10	11	→	9	1	9	10	14835.80664	-0.00017
9	3	7	9	→	8	3	6	8	14897.60894	0.00024
9	3	7	8	→	8	3	6	7	14897.72464	0.00067
9	3	7	10	→	8	3	6	9	14897.72464	0.00010
10	0	10	9	→	9	0	9	8	14903.23328	0.00240
10	0	10	10	→	9	0	9	9	14903.24547	0.00116
10	0	10	11	→	9	0	9	10	14903.24547	-0.00060
9	4	6	9	→	8	4	5	8	14928.11231	0.00024
9	4	6	10	→	8	4	5	9	14928.31864	0.00057
9	4	6	8	→	8	4	5	7	14928.33277	-0.00097
9	4	5	9	→	8	4	4	8	14956.38904	0.00031
9	4	5	10	→	8	4	4	9	14956.59873	0.00113
9	4	5	8	→	8	4	4	7	14956.61224	-0.00132
9	1	8	8	→	8	1	7	7	15078.40462	0.00024
9	1	8	10	→	8	1	7	9	15078.42422	-0.00063
9	1	8	9	→	8	1	7	8	15078.43019	0.00132
9	3	6	9	→	8	3	5	8	15248.85326	0.00041
9	3	6	10	→	8	3	5	9	15248.98748	0.00046
9	3	6	8	→	8	3	5	7	15248.98748	-0.00050
7	2	6	6	→	6	1	5	5	15491.34743	0.00036
7	2	6	8	→	6	1	5	7	15491.41764	-0.00011
7	2	6	7	→	6	1	5	6	15491.66934	-0.00075
9	2	7	9	→	8	2	6	8	15686.94359	0.00059
9	2	7	8	→	8	2	6	7	15686.98368	0.00126
9	2	7	10	→	8	2	6	9	15686.99476	-0.00082
10	2	9	10	→	9	2	8	9	15976.88668	0.00010
10	2	9	9	→	9	2	8	8	15976.90789	-0.00037
10	2	9	11	→	9	2	8	10	15976.91929	0.00006
11	0	11	10	→	10	1	10	9	16197.69644	-0.00112
11	0	11	11	→	10	1	10	10	16197.69664	0.00130

11	0	11	12	→	10	1	10	11	16197.70763	-0.00114
11	1	11	10	→	10	1	10	9	16262.56744	-0.00180
11	1	11	11	→	10	1	10	10	16262.57483	0.00131
11	1	11	12	→	10	1	10	11	16262.58299	0.00199
11	1	10	11	→	10	2	9	10	16274.98185	0.00004
11	1	10	10	→	10	2	9	9	16275.08500	0.00205
11	1	10	12	→	10	2	9	11	16275.08500	-0.00041
11	0	11	10	→	10	0	10	9	16305.21966	0.00025
11	0	11	11	→	10	0	10	10	16305.22857	-0.00037
11	0	11	12	→	10	0	10	11	16305.23258	0.00087
11	1	11	10	→	10	0	10	9	16370.09357	0.00249
11	1	11	12	→	10	0	10	11	16370.10405	0.00011
11	1	11	11	→	10	0	10	10	16370.10405	-0.00307
8	2	7	7	→	7	1	6	6	16421.14959	0.00078
8	2	7	9	→	7	1	6	8	16421.19990	-0.00034
8	2	7	8	→	7	1	6	7	16421.40305	-0.00001
10	3	8	10	→	9	3	7	9	16538.45137	0.00004
10	3	8	9	→	9	3	7	8	16538.52994	-0.00127
10	3	8	11	→	9	3	7	10	16538.53574	0.00088
10	1	9	9	→	9	1	8	8	16538.72311	0.00062
10	1	9	11	→	9	1	8	10	16538.73908	-0.00044
10	1	9	10	→	9	1	8	9	16538.74946	0.00037
10	4	7	10	→	9	4	6	9	16613.18578	0.00006
10	4	7	11	→	9	4	6	10	16613.33724	-0.00056
10	4	7	9	→	9	4	6	8	16613.34615	0.00126
10	4	6	10	→	9	4	5	9	16672.83825	-0.00026
10	4	6	11	→	9	4	5	10	16672.99530	-0.00011
10	4	6	9	→	9	4	5	8	16673.00474	0.00182
10	3	7	10	→	9	3	6	9	17085.56731	-0.00003
10	3	7	9	→	9	3	6	8	17085.67054	0.00216
10	3	7	11	→	9	3	6	10	17085.67054	-0.00016
9	2	8	8	→	8	1	7	7	17316.14152	-0.00076
9	2	8	10	→	8	1	7	9	17316.18118	0.00080
9	2	8	9	→	8	1	7	8	17316.34210	0.00042
10	2	8	10	→	9	2	7	9	17421.85242	-0.00019
10	2	8	9	→	9	2	7	8	17421.87253	-0.00020
10	2	8	11	→	9	2	7	10	17421.88554	0.00032
11	2	10	11	→	10	2	9	10	17479.01258	0.00075
11	2	10	10	→	10	2	9	9	17479.02304	-0.00163
11	2	10	12	→	10	2	9	11	17479.03457	0.00005
12	0	12	11	→	11	1	11	10	17646.65814	-0.00001
12	0	12	12	→	11	1	11	11	17646.65814	-0.00049
12	0	12	13	→	11	1	11	12	17646.66872	0.00093
12	1	12	11	→	11	1	11	10	17685.22104	-0.00177
12	1	12	12	→	11	1	11	11	17685.22741	0.00056
12	1	12	13	→	11	1	11	12	17685.23461	0.00188

12	0	12	11	→	11	0	11	10	17711.52787	-0.00196
12	0	12	12	→	11	0	11	11	17711.53766	0.00085
12	0	12	13	→	11	0	11	12	17711.54100	0.00098
12	1	12	11	→	11	0	11	10	17750.09349	-0.00099
12	1	12	13	→	11	0	11	12	17750.10520	0.00024
12	1	12	12	→	11	0	11	11	17750.10520	0.00016
11	1	10	10	→	10	1	9	9	17951.00734	0.00071
11	1	10	12	→	10	1	9	11	17951.02035	-0.00031
11	1	10	11	→	10	1	9	10	17951.03201	-0.00010
12	1	11	12	→	11	2	10	11	18129.18189	-0.00122
12	1	11	11	→	11	2	10	10	18129.24802	-0.00141
12	1	11	13	→	11	2	10	12	18129.25506	0.00144
11	3	9	11	→	10	3	8	10	18163.24508	0.00036
11	3	9	10	→	10	3	8	9	18163.29873	-0.00220
11	3	9	12	→	10	3	8	11	18163.30660	0.00066
11	6	6	11	→	10	6	5	10	18196.10541	0.00004
11	6	5	11	→	10	6	4	10	18196.31694	-0.00001
11	6	6	12	→	10	6	5	11	18196.35654	0.00093
11	6	6	10	→	10	6	5	9	18196.37748	-0.00053
11	6	5	12	→	10	6	4	11	18196.56749	0.00031
11	6	5	10	→	10	6	4	9	18196.58868	-0.00095
10	2	9	9	→	9	1	8	8	18214.64554	-0.00063
10	2	9	11	→	9	1	8	10	18214.67523	0.00046
10	2	9	10	→	9	1	8	9	18214.79978	0.00039
11	5	7	11	→	10	5	6	10	18246.67082	-0.00018
11	5	7	12	→	10	5	6	11	18246.84766	-0.00026
11	5	7	10	→	10	5	6	9	18246.85923	-0.00022
11	5	6	11	→	10	5	5	10	18253.39889	-0.00016
11	5	6	12	→	10	5	5	11	18253.57674	0.00013
11	5	6	10	→	10	5	5	9	18253.58755	-0.00064
11	4	8	11	→	10	4	7	10	18300.48787	0.00001
11	4	8	12	→	10	4	7	11	18300.60371	0.00056
11	4	8	10	→	10	4	7	9	18300.60371	-0.00170
11	4	7	11	→	10	4	6	10	18415.38677	-0.00036
11	4	7	12	→	10	4	6	11	18415.51089	0.00101
11	4	7	10	→	10	4	6	9	18415.51089	-0.00202
11	3	8	11	→	10	3	7	10	18946.12934	0.00141
11	3	8	10	→	10	3	7	9	18946.20140	-0.00254
11	3	8	12	→	10	3	7	11	18946.20902	0.00108
12	2	11	12	→	11	2	10	11	18962.22960	-0.00059
12	2	11	13	→	11	2	10	12	18962.24578	-0.00032
13	1	13	12	→	12	1	12	11	19105.10660	-0.00211
13	1	13	13	→	12	1	12	12	19105.11028	-0.00211
13	1	13	14	→	12	1	12	13	19105.11919	0.00201
11	2	9	11	→	10	2	8	10	19107.38134	-0.00080
11	2	9	10	→	10	2	8	9	19107.39115	0.00255

11	2	9	12	→	10	2	8	11	19107.39888	-0.00125
13	0	13	12	→	12	0	12	11	19121.02159	-0.00243
13	0	13	14	→	12	0	12	13	19121.03386	0.00124
12	1	11	11	→	11	1	10	10	19333.19173	0.00058
12	1	11	13	→	11	1	10	12	19333.20086	-0.00187
12	1	11	12	→	11	1	10	11	19333.21305	-0.00008
12	3	10	12	→	11	3	9	11	19768.66091	0.00009
12	3	10	11	→	11	3	9	10	19768.69861	-0.00193
12	3	10	13	→	11	3	9	12	19768.70751	0.00146
12	4	9	12	→	11	4	8	11	19986.72858	0.00059
12	4	9	13	→	11	4	8	12	19986.81716	-0.00008
12	4	9	11	→	11	4	8	10	19986.81716	-0.00015
12	4	8	12	→	11	4	7	11	20191.19259	-0.00037
12	4	8	13	→	11	4	7	12	20191.29300	0.00032
12	4	8	11	→	11	4	7	10	20191.29300	-0.00028
13	2	12	13	→	12	2	11	12	20428.75792	-0.00057
13	2	12	12	→	12	2	11	11	20428.76221	0.00021
13	2	12	14	→	12	2	11	13	20428.77054	0.00078
14	1	14	13	→	13	1	13	12	20523.20221	-0.00214
14	1	14	15	→	13	1	13	14	20523.21369	0.00204
14	0	14	13	→	13	0	13	12	20532.68340	-0.00229
14	0	14	15	→	13	0	13	14	20532.69457	0.00151
13	1	12	12	→	12	1	11	11	20703.61592	0.00133
13	1	12	14	→	12	1	11	13	20703.62231	-0.00187
13	1	12	13	→	12	1	11	12	20703.63247	0.00045
12	2	10	11	→	11	2	9	10	20735.11770	-0.00058
12	2	10	13	→	11	2	9	12	20735.13089	0.00186
12	3	9	12	→	11	3	8	11	20808.92440	-0.00011
12	3	9	11	→	11	3	8	10	20808.97888	-0.00141
12	3	9	13	→	11	3	8	12	20808.98606	0.00083
13	3	11	13	→	12	3	10	12	21352.25502	0.00079
13	3	11	12	→	12	3	10	11	21352.28075	-0.00139
13	3	11	14	→	12	3	10	13	21352.28843	0.00074
13	5	9	13	→	12	5	8	12	21635.25466	-0.00006
13	5	9	14	→	12	5	8	13	21635.36627	0.00169
13	5	9	12	→	12	5	8	11	21635.36627	-0.00150
13	5	8	13	→	12	5	7	12	21666.49289	-0.00067
13	5	8	14	→	12	5	7	13	21666.60692	0.00141
13	5	8	12	→	12	5	7	11	21666.60692	-0.00192
13	4	10	13	→	12	4	9	12	21667.88677	0.00045
13	4	10	12	→	12	4	9	11	21667.95509	0.00058
13	4	10	14	→	12	4	9	13	21667.95509	-0.00107
14	2	13	14	→	13	2	12	13	21881.27868	-0.00038
14	2	13	13	→	13	2	12	12	21881.27868	-0.00162
14	2	13	15	→	13	2	12	14	21881.28910	0.00193
15	1	15	14	→	14	1	14	13	21940.17915	0.00015

15	1	15	16	→	14	1	14	15	21940.18591	0.00055
15	0	15	14	→	14	0	14	13	21945.75635	-0.00057
15	0	15	15	→	14	0	14	14	21945.76293	0.00264
15	0	15	16	→	14	0	14	15	21945.76293	-0.00038
13	4	9	13	→	12	4	8	12	22006.27978	0.00063
13	4	9	12	→	12	4	8	11	22006.36219	0.00017
13	4	9	14	→	12	4	8	13	22006.36219	-0.00056
14	1	13	13	→	13	1	12	12	22075.22353	-0.00263
14	1	13	15	→	13	1	12	14	22075.23445	0.00029
14	1	13	14	→	13	1	12	13	22075.24019	0.00101
13	2	11	12	→	12	2	10	11	22298.07481	-0.00248
13	2	11	14	→	12	2	10	13	22298.08830	0.00174
13	2	11	13	→	12	2	10	12	22298.08830	-0.00036
13	3	10	13	→	12	3	9	12	22651.06800	0.00042
13	3	10	12	→	12	3	9	11	22651.10538	-0.00113
13	3	10	14	→	12	3	9	13	22651.11294	0.00100
14	3	12	14	→	13	3	11	13	22912.59972	0.00289
14	3	12	13	→	13	3	11	12	22912.61446	-0.00165
14	3	12	15	→	13	3	11	14	22912.62250	0.00101
15	2	14	14	→	14	2	13	13	23322.61097	-0.00054
15	2	14	15	→	14	2	13	14	23322.61097	-0.00065
15	2	14	16	→	14	2	13	15	23322.61894	0.00135

Table VI(B). Microwave transitions of the $^{13}C_1$ isotopologue of 24DFBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	ν_{obs}	$\nu_{obs.-calc.}$
4	1	3	4	→	3	1	2	3	6964.66432	0.00031
4	1	3	3	→	3	1	2	2	6964.76372	0.00059
4	1	3	5	→	3	1	2	4	6964.82518	0.00031
5	1	5	5	→	4	1	4	4	7560.45013	-0.00034
5	1	5	4	→	4	1	4	3	7560.48930	-0.00103
5	1	5	6	→	4	1	4	5	7560.53435	0.00015
5	0	5	4	→	4	0	4	3	7863.53853	0.00041
5	0	5	6	→	4	0	4	5	7863.61388	0.00155
5	0	5	5	→	4	0	4	4	7863.61388	-0.00181
5	2	4	5	→	4	2	3	4	8152.17025	0.00027
5	2	4	6	→	4	2	3	5	8152.46447	0.00034
5	2	4	4	→	4	2	3	3	8152.49333	-0.00042
5	2	3	5	→	4	2	2	4	8480.45637	-0.00011
5	2	3	6	→	4	2	2	5	8480.77534	-0.00044
5	2	3	4	→	4	2	2	3	8480.80684	-0.00053
5	1	4	5	→	4	1	3	4	8666.05798	-0.00043
5	1	4	4	→	4	1	3	3	8666.09032	0.00139
5	1	4	6	→	4	1	3	5	8666.14024	0.00004
6	1	6	6	→	5	1	5	5	9035.74939	0.00141
6	1	6	5	→	5	1	5	4	9035.76087	-0.00141
6	1	6	7	→	5	1	5	6	9035.79655	-0.00017
6	0	6	5	→	5	0	5	4	9299.32073	0.00105
6	0	6	7	→	5	0	5	6	9299.36703	-0.00126
6	0	6	6	→	5	0	5	5	9299.37655	0.00106
6	2	4	6	→	5	2	3	5	10280.13023	-0.00025
6	2	4	5	→	5	2	3	4	10280.32447	0.00050
6	2	4	7	→	5	2	3	6	10280.32447	0.00025
6	1	5	6	→	5	1	4	5	10336.00421	-0.00180
6	1	5	5	→	5	1	4	4	10336.00992	0.00066
6	1	5	7	→	5	1	4	6	10336.05037	0.00122
7	1	7	7	→	6	1	6	6	10497.12849	-0.00112
7	1	7	6	→	6	1	6	5	10497.13433	0.00129
7	1	7	8	→	6	1	6	7	10497.16035	0.00040
7	0	7	6	→	6	0	6	5	10704.68769	-0.00035
7	0	7	8	→	6	0	6	7	10704.72204	-0.00062
7	0	7	7	→	6	0	6	6	10704.72926	0.00082
7	2	6	7	→	6	2	5	6	11331.07067	-0.00057
7	2	6	6	→	6	2	5	5	11331.16931	0.00122
7	2	6	8	→	6	2	5	7	11331.17824	0.00009
8	1	8	7	→	7	1	7	6	11946.13594	0.00043
8	1	8	8	→	7	1	7	7	11946.13594	-0.00104
8	1	8	9	→	7	1	7	8	11946.15685	0.00000

7	1	6	6	→	6	1	5	5	11964.21323	-0.00157
7	1	6	7	→	6	1	5	6	11964.22543	-0.00030
7	1	6	8	→	6	1	5	7	11964.24648	0.00028
8	0	8	7	→	7	0	7	6	12097.04488	-0.00085
8	0	8	9	→	7	0	7	8	12097.07210	0.00109
8	0	8	8	→	7	0	7	7	12097.07210	-0.00198
9	1	9	8	→	8	1	8	7	13384.87851	-0.00081
9	1	9	9	→	8	1	8	8	13384.88511	0.00221
9	1	9	10	→	8	1	8	9	13384.89556	-0.00096
9	0	9	8	→	8	0	8	7	13488.13353	0.00112
9	0	9	10	→	8	0	8	9	13488.15140	-0.00025
9	0	9	9	→	8	0	8	8	13488.15140	-0.00064

Table VI(C). Microwave transitions of the $^{13}C_2$ isotopologue of 24DFBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	ν_{obs}	$\nu_{obs.-calc.}$
4	1	3	4	→	3	1	2	3	6971.87379	-0.00020
4	1	3	3	→	3	1	2	2	6971.97311	0.00008
4	1	3	5	→	3	1	2	4	6972.03572	0.00089
5	1	5	5	→	4	1	4	4	7563.78536	-0.00047
5	1	5	4	→	4	1	4	3	7563.82570	0.00007
5	1	5	6	→	4	1	4	5	7563.86975	0.00022
5	0	5	4	→	4	0	4	3	7866.24022	0.00031
5	0	5	6	→	4	0	4	5	7866.31538	0.00121
5	0	5	5	→	4	0	4	4	7866.31538	-0.00235
5	2	4	5	→	4	2	3	4	8158.60416	0.00042
5	2	4	6	→	4	2	3	5	8158.89799	0.00002
5	2	4	4	→	4	2	3	3	8158.92765	0.00007
5	2	3	5	→	4	2	2	4	8491.19719	0.00015
5	2	3	6	→	4	2	2	5	8491.51626	-0.00037
5	2	3	4	→	4	2	2	3	8491.54831	0.00009
5	1	4	5	→	4	1	3	4	8674.42123	-0.00065
5	1	4	4	→	4	1	3	3	8674.45300	0.00077
5	1	4	6	→	4	1	3	5	8674.50373	0.00018
6	1	6	6	→	5	1	5	5	9039.31781	0.00030
6	1	6	5	→	5	1	5	4	9039.33073	-0.00101
6	1	6	7	→	5	1	5	6	9039.36568	-0.00053
6	0	6	5	→	5	0	5	4	9301.39614	0.00078
6	0	6	7	→	5	0	5	6	9301.44288	-0.00111
6	0	6	6	→	5	0	5	5	9301.45200	0.00074
6	2	4	5	→	5	2	3	4	10293.87350	-0.00001
6	2	4	7	→	5	2	3	6	10293.87350	-0.00029
6	1	5	6	→	5	1	4	5	10344.97718	-0.00124
6	1	5	5	→	5	1	4	4	10344.98123	-0.00018
6	1	5	7	→	5	1	4	6	10345.02185	0.00050
7	1	7	7	→	6	1	6	6	10500.82758	0.00039
7	1	7	6	→	6	1	6	5	10500.83132	0.00075
7	1	7	8	→	6	1	6	7	10500.85780	0.00030
7	0	7	6	→	6	0	6	5	10706.38174	0.00059
7	0	7	8	→	6	0	6	7	10706.41465	-0.00109
7	0	7	7	→	6	0	6	6	10706.42247	0.00098
7	2	6	7	→	6	2	5	6	11338.89772	-0.00043
7	2	6	6	→	6	2	5	5	11338.99623	0.00129
7	2	6	8	→	6	2	5	7	11339.00485	-0.00017
8	1	8	7	→	7	1	7	6	11949.90282	-0.00013
8	1	8	8	→	7	1	7	7	11949.90282	-0.00163
8	1	8	9	→	7	1	7	8	11949.92440	0.00010
7	1	6	6	→	6	1	5	5	11973.07557	-0.00018

7	1	6	7	→	6	1	5	6	11973.08669	-0.00032
7	1	6	8	→	6	1	5	7	11973.10735	0.00016
8	0	8	7	→	7	0	7	6	12098.73928	-0.00052
8	0	8	9	→	7	0	7	8	12098.76643	0.00137
8	0	8	8	→	7	0	7	7	12098.76643	-0.00159
9	1	9	8	→	8	1	8	7	13388.70223	-0.00067
9	1	9	9	→	8	1	8	8	13388.70818	0.00168
9	1	9	10	→	8	1	8	9	13388.71914	-0.00097
9	0	9	8	→	8	0	8	7	13490.12724	0.00062
9	0	9	10	→	8	0	8	9	13490.14558	-0.00027
9	0	9	9	→	8	0	8	8	13490.14558	-0.00052

Table VI(D). Microwave transitions of the $^{13}C_3$ isotopologue of 24DFBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	ν_{obs}	$\nu_{obs.-calc.}$
4	1	3	4	→	3	1	2	3	6958.81016	-0.00024
4	1	3	3	→	3	1	2	2	6958.90830	-0.00105
4	1	3	5	→	3	1	2	4	6958.97211	0.00066
5	1	5	5	→	4	1	4	4	7549.58887	-0.00030
5	1	5	4	→	4	1	4	3	7549.62676	-0.00223
5	1	5	6	→	4	1	4	5	7549.67260	-0.00028
5	0	5	4	→	4	0	4	3	7851.46973	0.00042
5	0	5	6	→	4	0	4	5	7851.54431	0.00056
5	0	5	5	→	4	0	4	4	7851.54431	-0.00345
5	2	4	5	→	4	2	3	4	8143.30584	0.00038
5	2	4	6	→	4	2	3	5	8143.60063	0.00048
5	2	4	4	→	4	2	3	3	8143.63004	0.00024
5	2	3	5	→	4	2	2	4	8475.29910	0.00024
5	2	3	6	→	4	2	2	5	8475.61953	0.00014
5	2	3	4	→	4	2	2	3	8475.65086	-0.00021
5	1	4	5	→	4	1	3	4	8658.16441	-0.00035
5	1	4	4	→	4	1	3	3	8658.19572	0.00082
5	1	4	6	→	4	1	3	5	8658.24596	-0.00048
6	1	6	6	→	5	1	5	5	9022.34982	0.00078
6	1	6	5	→	5	1	5	4	9022.36281	-0.00040
6	1	6	7	→	5	1	5	6	9022.39716	-0.00052
6	0	6	5	→	5	0	5	4	9283.92423	0.00057
6	0	6	7	→	5	0	5	6	9283.97154	-0.00086
6	0	6	6	→	5	0	5	5	9283.98049	0.00038
6	2	4	6	→	5	2	3	5	10274.41059	0.00011
6	2	4	5	→	5	2	3	4	10274.60490	0.00020
6	2	4	7	→	5	2	3	6	10274.60490	-0.00007
6	1	5	6	→	5	1	4	5	10325.58325	-0.00125
6	1	5	5	→	5	1	4	4	10325.58325	-0.00395
6	1	5	7	→	5	1	4	6	10325.62849	0.00119
7	1	7	7	→	6	1	6	6	10481.11100	-0.00161
7	1	7	6	→	6	1	6	5	10481.11631	0.00042
7	1	7	8	→	6	1	6	7	10481.14293	0.00010
7	0	7	6	→	6	0	6	5	10686.26814	0.00145
7	0	7	8	→	6	0	6	7	10686.30004	-0.00130
7	0	7	7	→	6	0	6	6	10686.30785	0.00037
7	2	6	7	→	6	2	5	6	11317.63041	-0.00019
7	2	6	6	→	6	2	5	5	11317.72904	0.00162
7	2	6	8	→	6	2	5	7	11317.73764	0.00011
8	1	8	7	→	7	1	7	6	11927.46696	0.00179
8	1	8	8	→	7	1	7	7	11927.46696	0.00018
8	1	8	9	→	7	1	7	8	11927.48657	0.00004

7	1	6	6	→	6	1	5	5	11950.62007	0.00000
7	1	6	7	→	6	1	5	6	11950.63173	0.00003
7	1	6	8	→	6	1	5	7	11950.65209	0.00045
8	0	8	7	→	7	0	7	6	12076.00731	-0.00142
8	0	8	9	→	7	0	7	8	12076.03626	0.00222
8	0	8	8	→	7	0	7	7	12076.03626	-0.00104
9	1	9	8	→	8	1	8	7	13363.56020	-0.00109
9	1	9	9	→	8	1	8	8	13363.56738	0.00238
9	1	9	10	→	8	1	8	9	13363.57743	-0.00108
9	0	9	8	→	8	0	8	7	13464.78378	0.00117
9	0	9	10	→	8	0	8	9	13464.80201	0.00014
9	0	9	9	→	8	0	8	8	13464.80201	-0.00035

Table VI(E). Microwave transitions of the $^{13}C_4$ isotopologue of 24DFBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	ν_{obs}	$\nu_{obs.-calc.}$
4	1	3	4	→	3	1	2	3	6934.73202	-0.00226
4	1	3	3	→	3	1	2	2	6934.83455	0.00032
4	1	3	5	→	3	1	2	4	6934.89567	-0.00022
5	1	5	5	→	4	1	4	4	7533.23488	0.00120
5	1	5	4	→	4	1	4	3	7533.27555	0.00172
5	1	5	6	→	4	1	4	5	7533.31786	-0.00009
5	0	5	4	→	4	0	4	3	7836.10841	-0.00119
5	0	5	6	→	4	0	4	5	7836.18491	0.00093
5	0	5	5	→	4	0	4	4	7836.18491	-0.00161
5	2	4	5	→	4	2	3	4	8119.49500	0.00138
5	2	4	6	→	4	2	3	5	8119.78919	0.00026
5	2	4	4	→	4	2	3	3	8119.81991	0.00121
5	2	3	5	→	4	2	2	4	8441.74321	0.00025
5	2	3	6	→	4	2	2	5	8442.06237	-0.00027
5	2	3	4	→	4	2	2	3	8442.09448	0.00018
5	1	4	5	→	4	1	3	4	8629.52126	-0.00069
5	1	4	4	→	4	1	3	3	8629.55344	0.00029
5	1	4	6	→	4	1	3	5	8629.60361	-0.00078
6	1	6	6	→	5	1	5	5	9003.70823	0.00067
6	1	6	5	→	5	1	5	4	9003.72034	-0.00176
6	1	6	7	→	5	1	5	6	9003.75530	-0.00143
6	0	6	5	→	5	0	5	4	9268.20836	0.00095
6	0	6	7	→	5	0	5	6	9268.25470	-0.00143
6	0	6	6	→	5	0	5	5	9268.26360	0.00089
6	2	4	6	→	5	2	3	5	10232.56311	-0.00011
6	2	4	5	→	5	2	3	4	10232.75709	0.00014
6	2	4	7	→	5	2	3	6	10232.75709	-0.00009
6	1	5	6	→	5	1	4	5	10293.58848	-0.00204
6	1	5	5	→	5	1	4	4	10293.59423	-0.00023
6	1	5	7	→	5	1	4	6	10293.63622	0.00189
7	1	7	7	→	6	1	6	6	10460.43307	-0.00087
7	1	7	6	→	6	1	6	5	10460.43889	0.00131
7	1	7	8	→	6	1	6	7	10460.46482	0.00019
7	0	7	6	→	6	0	6	5	10669.71148	0.00068
7	0	7	8	→	6	0	6	7	10669.74423	-0.00136
7	0	7	7	→	6	0	6	6	10669.75187	0.00095
7	2	6	7	→	6	2	5	6	11286.95186	0.00024
7	2	6	6	→	6	2	5	5	11287.04982	0.00073
7	2	6	8	→	6	2	5	7	11287.05899	-0.00016
8	1	8	7	→	7	1	7	6	11904.89330	0.00051
8	1	8	8	→	7	1	7	7	11904.89330	-0.00077
8	1	8	9	→	7	1	7	8	11904.91364	-0.00060

7	1	6	6	→	6	1	5	5	11916.88764	0.00228
7	1	6	7	→	6	1	5	6	11916.89460	-0.00090
7	1	6	8	→	6	1	5	7	11916.91647	-0.00026
8	0	8	7	→	7	0	7	6	12057.79349	-0.00166
8	0	8	9	→	7	0	7	8	12057.82260	0.00205
8	0	8	8	→	7	0	7	7	12057.82260	-0.00076
9	1	9	8	→	8	1	8	7	13339.13809	-0.00077
9	1	9	9	→	8	1	8	8	13339.14320	0.00092
9	1	9	10	→	8	1	8	9	13339.15479	-0.00136
9	0	9	8	→	8	0	8	7	13444.25716	0.00172
9	0	9	10	→	8	0	8	9	13444.27469	-0.00010
9	0	9	9	→	8	0	8	8	13444.27469	-0.00032

Table VI(F). Microwave transitions of the $^{13}C_5$ isotopologue of 24DFBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	ν_{obs}	$\nu_{obs.-calc.}$
4	1	3	4	→	3	1	2	3	6949.44398	-0.00050
4	1	3	3	→	3	1	2	2	6949.54375	0.00043
4	1	3	5	→	3	1	2	4	6949.60472	-0.00036
5	1	5	5	→	4	1	4	4	7535.56625	0.00005
5	1	5	4	→	4	1	4	3	7535.60577	-0.00013
5	1	5	6	→	4	1	4	5	7535.65038	0.00061
5	0	5	4	→	4	0	4	3	7836.21091	0.00130
5	0	5	6	→	4	0	4	5	7836.28505	0.00123
5	0	5	5	→	4	0	4	4	7836.28505	-0.00251
5	2	4	5	→	4	2	3	4	8130.62305	0.00000
5	2	4	6	→	4	2	3	5	8130.91701	0.00004
5	2	4	4	→	4	2	3	3	8130.94641	-0.00013
5	2	3	5	→	4	2	2	4	8465.60331	0.00015
5	2	3	6	→	4	2	2	5	8465.92277	0.00015
5	2	3	4	→	4	2	2	3	8465.95385	-0.00033
5	1	4	5	→	4	1	3	4	8645.98196	-0.00048
5	1	4	4	→	4	1	3	3	8646.01380	0.00121
5	1	4	6	→	4	1	3	5	8646.06381	-0.00008
6	1	6	6	→	5	1	5	5	9005.23093	0.00057
6	1	6	5	→	5	1	5	4	9005.24327	-0.00125
6	1	6	7	→	5	1	5	6	9005.27872	-0.00024
6	0	6	5	→	5	0	5	4	9264.92363	0.00108
6	0	6	7	→	5	0	5	6	9264.97023	-0.00091
6	0	6	6	→	5	0	5	5	9264.97967	0.00121
6	2	4	6	→	5	2	3	5	10263.10052	-0.00016
6	2	4	5	→	5	2	3	4	10263.29413	0.00012
6	2	4	7	→	5	2	3	6	10263.29413	-0.00019
6	1	5	6	→	5	1	4	5	10310.18129	-0.00148
6	1	5	5	→	5	1	4	4	10310.18585	0.00032
6	1	5	7	→	5	1	4	6	10310.22695	0.00149
7	1	7	7	→	6	1	6	6	10460.83768	-0.00114
7	1	7	6	→	6	1	6	5	10460.84255	0.00040
7	1	7	8	→	6	1	6	7	10460.86930	0.00024
7	0	7	6	→	6	0	6	5	10663.80885	0.00033
7	0	7	8	→	6	0	6	7	10663.84120	-0.00183
7	0	7	7	→	6	0	6	6	10663.84948	0.00073
7	2	6	7	→	6	2	5	6	11299.03536	-0.00032
7	2	6	6	→	6	2	5	5	11299.13296	0.00066
7	2	6	8	→	6	2	5	7	11299.14248	0.00011
8	1	8	7	→	7	1	7	6	11904.01589	0.00077
8	1	8	8	→	7	1	7	7	11904.01589	-0.00076
8	1	8	9	→	7	1	7	8	11904.03685	0.00040

7	1	6	6	→	6	1	5	5	11931.46535	-0.00205
7	1	6	7	→	6	1	5	6	11931.47967	0.00073
7	1	6	8	→	6	1	5	7	11931.49941	0.00057
8	0	8	7	→	7	0	7	6	12050.45232	-0.00094
8	0	8	9	→	7	0	7	8	12050.47913	0.00066
8	0	8	8	→	7	0	7	7	12050.47913	-0.00220
9	1	9	8	→	8	1	8	7	13336.94682	-0.00037
9	1	9	9	→	8	1	8	8	13336.95225	0.00144
9	1	9	10	→	8	1	8	9	13336.96346	-0.00093
9	0	9	8	→	8	0	8	7	13436.38753	0.00132
9	0	9	10	→	8	0	8	9	13436.40525	-0.00015
9	0	9	9	→	8	0	8	8	13436.40525	-0.00030

Table VI(G). Microwave transitions of the $^{13}C_6$ isotopologue of 24DFBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	ν_{obs}	$\nu_{obs.-calc.}$
4	1	3	4	→	3	1	2	3	6968.64224	-0.00038
4	1	3	3	→	3	1	2	2	6968.74186	0.00043
4	1	3	5	→	3	1	2	4	6968.80341	-0.00017
5	1	5	5	→	4	1	4	4	7551.08321	-0.00027
5	1	5	4	→	4	1	4	3	7551.12309	-0.00008
5	1	5	6	→	4	1	4	5	7551.16686	-0.00029
5	0	5	4	→	4	0	4	3	7851.39122	0.00071
5	0	5	5	→	4	0	4	4	7851.46931	-0.00003
5	2	4	6	→	4	2	3	5	8151.01685	0.00005
5	2	4	4	→	4	2	3	3	8151.04649	0.00005
5	1	4	5	→	4	1	3	4	8669.13028	-0.00077
5	1	4	4	→	4	1	3	3	8669.16310	0.00224
5	1	4	6	→	4	1	3	5	8669.21189	-0.00057
6	1	6	6	→	5	1	5	5	9023.27732	0.00032
6	1	6	5	→	5	1	5	4	9023.29064	-0.00041
6	1	6	7	→	5	1	5	6	9023.32547	-0.00011
6	0	6	5	→	5	0	5	4	9281.56537	0.00022
6	0	6	7	→	5	0	5	6	9281.61242	-0.00149
6	0	6	6	→	5	0	5	5	9281.62326	0.00161
6	2	4	6	→	5	2	3	5	10294.94001	0.00059
6	2	4	5	→	5	2	3	4	10295.13308	-0.00051
6	2	4	7	→	5	2	3	6	10295.13308	-0.00086
6	1	5	6	→	5	1	4	5	10336.57018	-0.00107
6	1	5	5	→	5	1	4	4	10336.57018	-0.00330
6	1	5	7	→	5	1	4	6	10336.61456	0.00091
7	1	7	7	→	6	1	6	6	10481.26797	-0.00153
7	1	7	6	→	6	1	6	5	10481.27316	0.00046
7	1	7	8	→	6	1	6	7	10481.29964	-0.00003
7	0	7	6	→	6	0	6	5	10682.17750	0.00105
7	0	7	8	→	6	0	6	7	10682.20948	-0.00154
7	0	7	7	→	6	0	6	6	10682.21758	0.00059
7	2	6	7	→	6	2	5	6	11325.62443	-0.00026
7	2	6	6	→	6	2	5	5	11325.72293	0.00153
7	2	6	8	→	6	2	5	7	11325.73212	0.00059
8	1	8	7	→	7	1	7	6	11926.74579	0.00088
8	1	8	8	→	7	1	7	7	11926.74579	-0.00079
8	1	8	9	→	7	1	7	8	11926.76653	0.00023
7	1	6	6	→	6	1	5	5	11960.15702	-0.00108
7	1	6	7	→	6	1	5	6	11960.17047	0.00014
7	1	6	8	→	6	1	5	7	11960.19004	0.00031
8	0	8	7	→	7	0	7	6	12070.98493	-0.00079
8	0	8	9	→	7	0	7	8	12071.01237	0.00139

8	0	8	8	→	7	0	7	7	12071.01237	-0.00156
9	1	9	8	→	8	1	8	7	13361.94709	-0.00055
9	1	9	9	→	8	1	8	8	13361.95268	0.00132
9	1	9	10	→	8	1	8	9	13361.96406	-0.00081
9	0	9	8	→	8	0	8	7	13459.42746	0.00083
9	0	9	10	→	8	0	8	9	13459.44583	-0.00002
9	0	9	9	→	8	0	8	8	13459.44583	-0.00019

Table VI(H). Microwave transitions of the $^{13}C_7$ isotopologue of 24DFBN in MHz

J'	Ka'	Kc'	F'	→	J"	Ka"	Kc"	F"	ν_{obs}	$\nu_{obs.-calc.}$
4	1	3	4	→	3	1	2	3	6909.23163	-0.00005
4	1	3	3	→	3	1	2	2	6909.33296	0.00158
4	1	3	5	→	3	1	2	4	6909.39369	0.00065
5	1	5	5	→	4	1	4	4	7507.66187	0.00030
5	1	5	4	→	4	1	4	3	7507.70167	0.00000
5	1	5	6	→	4	1	4	5	7507.74563	-0.00003
5	0	5	4	→	4	0	4	3	7809.85557	0.00001
5	0	5	6	→	4	0	4	5	7809.93022	0.00038
5	0	5	5	→	4	0	4	4	7809.93022	-0.00230
5	2	4	6	→	4	2	3	5	8090.88288	0.00031
5	2	4	4	→	4	2	3	3	8090.91234	0.00005
5	2	3	6	→	4	2	2	5	8410.11199	-0.00082
5	2	3	4	→	4	2	2	3	8410.14377	-0.00067
5	1	4	5	→	4	1	3	4	8598.06794	-0.00036
5	1	4	4	→	4	1	3	3	8598.09979	0.00041
5	1	4	6	→	4	1	3	5	8598.15026	-0.00034
6	1	6	6	→	5	1	5	5	8973.34001	0.00029
6	1	6	5	→	5	1	5	4	8973.35354	-0.00069
6	1	6	7	→	5	1	5	6	8973.38841	-0.00035
6	0	6	5	→	5	0	5	4	9237.69330	0.00058
6	0	6	7	→	5	0	5	6	9237.74032	-0.00105
6	0	6	6	→	5	0	5	5	9237.74916	0.00101
6	2	4	6	→	5	2	3	5	10193.57264	-0.00023
6	2	4	5	→	5	2	3	4	10193.76728	0.00080
6	2	4	7	→	5	2	3	6	10193.76728	0.00058
6	1	5	6	→	5	1	4	5	10256.53361	-0.00182
6	1	5	5	→	5	1	4	4	10256.54051	0.00118
6	1	5	7	→	5	1	4	6	10256.58019	0.00102
7	1	7	7	→	6	1	6	6	10425.36341	-0.00168
7	1	7	6	→	6	1	6	5	10425.36999	0.00129
7	1	7	8	→	6	1	6	7	10425.39561	-0.00007
7	0	7	6	→	6	0	6	5	10634.92634	0.00062
7	0	7	8	→	6	0	6	7	10634.95919	-0.00131
7	0	7	7	→	6	0	6	6	10634.96684	0.00081
7	2	6	7	→	6	2	5	6	11247.28952	0.00019
7	2	6	6	→	6	2	5	5	11247.38649	-0.00012
7	2	6	8	→	6	2	5	7	11247.39700	0.00034
8	1	8	7	→	7	1	7	6	11865.19168	0.00100
8	1	8	8	→	7	1	7	7	11865.19168	-0.00033
8	1	8	9	→	7	1	7	8	11865.21255	0.00046
7	1	6	6	→	6	1	5	5	11874.69102	-0.00161
7	1	6	7	→	6	1	5	6	11874.70265	-0.00014

7	1	6	8	→	6	1	5	7	11874.72451	0.00054
8	0	8	7	→	7	0	7	6	12018.60116	-0.00129
8	0	8	9	→	7	0	7	8	12018.63059	0.00276
8	0	8	8	→	7	0	7	7	12018.63059	-0.00026
9	1	9	8	→	8	1	8	7	13294.84347	-0.00041
9	1	9	9	→	8	1	8	8	13294.84907	0.00172
9	1	9	10	→	8	1	8	9	13294.85985	-0.00129
9	0	9	8	→	8	0	8	7	13400.51561	0.00084
9	0	9	10	→	8	0	8	9	13400.53342	-0.00067
9	0	9	9	→	8	0	8	8	13400.53342	-0.00109

Table VI(I). Microwave transitions of the ^{15}N isotopologue of 24DFBN in MHz

J'	K_a'	K_c'	→	J"	K_a"	K_c"	$\nu_{obs.}$	$\nu_{obs.-calc.}$
4	1	3	→	3	1	2	6831.80393	-0.00054
5	1	5	→	4	1	4	7433.92785	0.00026
5	0	5	→	4	0	4	7734.79912	-0.00045
5	2	4	→	4	2	3	8004.69731	0.00021
5	2	3	→	4	2	2	8311.30424	-0.00020
5	1	4	→	4	1	3	8502.99404	0.00004
6	1	6	→	5	1	5	8886.13466	0.00052
6	0	6	→	5	0	5	9151.54259	-0.00019
6	2	5	→	5	2	4	9575.41265	-0.00031
6	2	4	→	5	2	3	10072.72080	0.00005
6	1	5	→	5	1	4	10145.32403	0.00005
7	1	7	→	6	1	6	10325.07166	-0.00012
7	0	7	→	6	0	6	10537.46582	0.00073
7	2	6	→	6	2	5	11130.18878	0.00023
7	1	6	→	6	1	5	11749.33184	-0.00009
8	1	8	→	7	1	7	11752.06838	-0.00021
7	2	5	→	6	2	4	11847.27008	0.00031
8	0	8	→	7	0	7	11909.07783	-0.00026
8	2	7	→	7	2	6	12667.11399	-0.00045
9	1	9	→	8	1	8	13169.02881	-0.00019
9	0	9	→	8	0	8	13278.21865	0.00005
8	1	7	→	7	1	6	13305.33771	0.00024
9	2	8	→	8	2	7	14184.87836	0.00015