Supplementary Material

# Benchmarking a new segmented K-band chirped-pulse microwave spectrometer and its application to the conformationally rich amino alcohol isoleucinol

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## Contents

## S1 Instrument Design

In this work, we present a new design for chirped pulse Fourier transform microwave (CP-FTMW) spectrometers with the intention of reducing the cost required to construct such an instrument, thereby making the technique more accessible to academic and research institutions. By implementing the segmented approach that was developed for the millimeter wave (mmw) regime and coupling it with high-speed, state-of-the-art electronics, segmented CP-FTMW spectrometers can be built for half the cost while still retaining the performance capabilities of direct excitation and direct detection CP-FTMW spectrometers. In what follows, a more detailed description of the instrument, the schematic of which is found in Fig. 1 of the manuscript, is given, along with performance metrics.

### S1.1 AWG waveforms

In direct pulse excitation and detection CP-FTMWs, high cost arbitrary waveform generators (AWGs) and oscilloscopes are required to produce pulses and to digitize free inductin decays (FIDs), respectively, that span the entire bandwidth of the instrument. This is especially true when talking about instruments that operate at frequencies higher than 10 GHz, as AWGs and oscilloscopes with digitization rates of more than 25 GS/s are necessary. In order to combat this problem, especially up in the millimeter wave (mmw) regime where the availability and cost of electronics become a challenge, the segmented chirped pulse technique was implemented[1,2]. In this technique, the entire bandwidth of the spectrometer is divided into multiple small bandwidth sections and excited sequentially. The smaller bandwidth pulses allow for the use of less costly, lower bandwidth electronics; however, in the case of the AWG, high spectral purity is still needed to avoid introducing a multitude of spurious signals. These pulses can be up-converted to the desired measurement frequency range, and the molecular signals can be down-converted to a frequency range that fits within the requirements of the oscilloscope[1,2]. In the case of the presented 18-26 GHz spectrometer, the entire 8 GHz of bandwidth is divided into 10 segments, each with a final bandwidth of 800 MHz. A conceptual depiction of this can be seen in Fig. S1. In the AWG, the waveform consists of the first 1.5 $\mu$s pulse (covering 18.0-18.8 GHz after up-conversion) followed by 13.5 $\mu$s of deadtime and then the second pulse followed by deadtime. This is repeated until all 10 segments have been covered. The resulting waveform is referred to as a pulse train.

While this method increases the measurement time needed to collect one acquisition across the entire bandwidth, it has been demonstrated that the time required to achieve a spectrum with the same signal-to-noise ratio (SNR) for both a segmented collection and broadband collection is the same. By dividing the bandwidth into N segments, the excitation

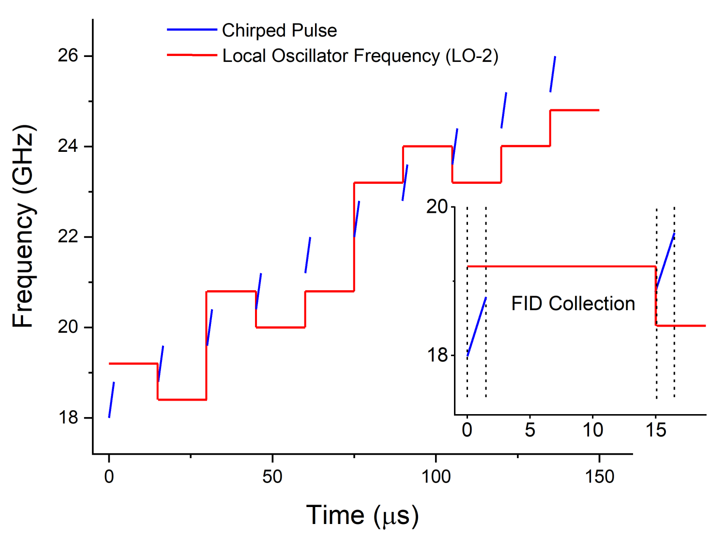


Fig. S1 Conceptual segmented 18-26 GHz CP-FTMW spectrogram of the chirped pulses and LO-2 frequencies. The blue trace is the sequence of 800 MHz bandwidth chirped pulses, 1.5 $\mu$s in duration, which are used to excite the molecular ensemble. Simultaneously, the LO-2 frequencies (red trace) down-converts the FID signals before it can be digitized on a 3.2 GS/s digitizer card.

bandwidth of the each segment decreases by a factor of N and the power/frequency increases by $\sqrt{N}$. As we are working in the weak pulse limit, the absolute intensity of each rotational transition increases by the $\sqrt{N}$ compared to a broadband acquisition. In general the SNR of a spectrum can be increased by the factor of the square root of the number of spectral acquisitions. Thus, to recover the factor of $\sqrt{N}$ that the segmented spectrum gained, N spectral acquisitions must be acquired in the broadband measurement[1].

In order to increase the acquisition of data, the multi-train method has been implemented. This is complementary to the fast frame option that is enabled in the Hamburg COMPACT spectrometer. The COMPACT spectrometer operates between 2-8 GHz, and each experiment cycle (frame) is 45 $\mu$s long. By enabling the fast frame option the experiment can be setup to allow for multiple frames to be included per gas pulse. Presently, the Hamburg COMPACT spectrometer can include eight frames per gas pulse. In the segmented 18-26 GHz CP-FTMW spectrometer, we have included the multi-frame option, which makes use of the large AWG memory capacity. This acts like fast frame, in that multiple pulse trains are generated back to back, and they collect data from the same gas pulse. In the current setup, the final AWG waveform consists of a series of three pulse trains or 30 chirped-pulse segments. The first 10 segments belong to the first pulse train, the next 10 segments to the second pulse train, and the last 10 segments to the third pulse train. In principle, more pulse trains can be added to the waveform if the gas pulse duration were to increase. With the multi-train method, the FID collection time is increased by a factor of three, and it allows us to record around 2.5 million averages in a day.

### S1.2 Excitation Pulse Generation

A dual channel 25 GS/s per channel arbitrary waveform generator (AWG, Textronix AWG70000A series) is used to create the series of excitation pulse trains (via CH1) and the series of local oscillator pulses (via CH2). This AWG was chosen due its high spurious and harmonic suppression. The chirps from CH1 span the frequency range 7-3 GHz in 10 segments where each segment of 15 $\mu$s has a 1.5 $\mu$s chirp covering 400 MHz of bandwidth (for example, chirps spanning 7-6.6 GHz, 6.6–6.2 GHz, and so on). This pulse train is then up-converted by mixing with a 16 GHz single frequency local oscillator (LO-1) pulse, as can be seen in Fig. 1. The generation of LO-1 is described later in this section.

The outputs from AWG CH1 and LO-1 are fed into M1 (Marki T320LS-1521), which is a two-tone-terminator mixer. The lower sideband of this mixing stage is selected by a bandpass filter (Lorch 9IZ7-11000/4000S) to obtain pulses that range between 9-13 GHz. After filtering, each segment of the pulse train is amplified (Marki A-0126EZP5-1523) and doubled (Marki MLD0632LS-1452), where the doubler multiplies both the frequency and the bandwidth of the pulse train by two without changing the pulse duration. A bandpass filter (Reactel 9CX11-22G-X8G S11) allows frequencies between 18-26 GHz to pass through, after which the series of pulse trains is amplified using a solid state amplifier (SSA) from Quinstar (QPP-18273840MPI) by approximately 6 W. The SSA is equipped with an internal switch so that random signals (noise) coming from the SSA after the pulse passes through can be blocked. The switch has pulse modulation TTL time of 2 $\mu$s, which is longer than the experimentally determined optimal pulse duration of 1.5 $\mu$s. Therefore, in order to block these random signals of the SSA when using pulse durations of 1.5 $\mu$s, a Single-Pole-Single-Throw (SPST) switch (Kratos Microwave Electronics Division F9012) has been implemented after the SSA. The microwave pulse train series is then broadcast across the vacuum chamber using an ATM microwave 20 dB gain horn antenna (Model number 42-442-6) which is separated by 20 cm from the same model receiver antenna.

As shown in subset LO-1 in Fig. 1, the single frequency 16 GHz LO-1 pulse is created by quadrupling (Quadrupler - Marki AQA-1933), amplifying (Minicircuits, ZRON-8G+) and doubling (Doubler - Eclipse D2010LZ1) a 2 GHz pulse generated by a Valon synthesizer (Valon Technology 5008 Dual Frequency Synthesizer). Cavity filters are used at each stage to remove harmonics and sideband signals from the LO-1 pulse (2 GHz - DBWAVE DBBF0402000200A, 8 GHz - DBWAVE DBBF0408000800B, 16 GHz – Lorch 2CF7-16000/80-S). The 16 GHz LO-1 pulse is then amplified (Minicircuits, ZVA-183+) and passed through a power divider (Minicircuits ZX10-2-183-S+) to mix with the output of CH1 and CH2.

### S1.3 FID Collection and Down-conversion

The receiver antenna collects the high power excitation pulses and the FID of the molecular sample. The excitation pulses are blocked by an SPST switch (American Microwave Corporation SWCH1K-Dc40-SK), and only the FIDs are allowed to pass. These FIDs are amplified by two low noise amplifiers (LNA) operating from 14-27 GHz (Hittite HMC504LC4B, Noise Figure: 2.2 dB @ 20 GHz) and 17-27 GHz (Hittite HMC751LC4, Noise Figure: 2.2 dB), and then they are down-converted to 400-1200 MHz. This occurs by mixing (M3, Marki M20240LP) the FIDs with a local oscillator pulse (LO-2). The generation of LO-2 is explained below. The intermediate frequency (IF) output of M3 spans 400-1200 MHz for each segment and is digitized on a 3.2 GS/s digitizer card (Keysight U5303A). This digitizer card is a 12-bit PCIe signal acquisition card, with an on-board data processing unit using a Xilinx Field Programmable Gate Array (FPGA), and it can perform real time averaging. The duration of the pulse train has been optimized so that the entirety of the FPGA memory will be filled in one acquisition. At 3.2 GS/s, this results in 150 $\mu$s. Thus, the digitizer card acquires the entire 150 $\mu$s with a single oscilloscope trigger, after which it requires 500 ns as a re-arm time before being able to accept the next trigger. This card also has a 4 GB DDR3 on-board memory, which dictates the number of averages the card can acquire before having to transfer the data to the PC. With the present card, a maximum of up to 500 000 averages can be processed on the card during the experiment before being transferred.

The second channel (CH2) of the AWG is used to create a series of pulse trains (subset LO-2, Fig. 1) between 7-3 GHz, in which the pulses are single frequency. The output of CH2 is up-converted by mixing (M2, same as M1) with LO-1. In a similar way to the excitation pulse train creation, the lower sidebands of this mixing stage are selected, amplified, doubled, and again filtered to only allow frequencies between 18-26 GHz to pass through. The final single frequency pulses are amplified (Marki A-0126EZP5-1534) and passed through the triple balanced mixer (M3) to down-convert the FID signals. The amplification step before the mixing stage is necessary to meet the minimum power for the mixer (M3).

The resulting LO-2 pulse train consists of 10 single-frequency sine waves, which each coincide with a segment in CH1 at an offset of 400 MHz above the end (for segments 1, 3, 6 and 7) or below the start (for segments 2, 4, 5, 8, 9 and 10) of the corresponding chirp. The mixing from above or below was chosen to decrease spurious signal generated by electronics for each segment. A conceptual spectrogram of the up-converted outputs of the two AWG waveforms is presented in Fig. S1.

### S1.4 Phase Locking and spectrum generation

The AWG is phase locked with the Valon synthesizer by using the internal 10 MHz temperature compensated crystal oscillator (TCXO) of the Valon synthesizer. A clock distribution board (Digikey AD9513/PCBZ-ND) takes the TCXO reference as its input and one of its outputs is used to phase lock the AWG. The SSA, digitizer card, and SPST switches are triggered with the four marker channels of the AWG. The delay between the valve driver for the molecular pulse and the pulse generation of the AWG is controlled using a delay generator (Stanford Research Systems DG 645), as shown in Fig. 1.

The signal is processed by extracting 10 $\mu$s of the FID from each segment, beginning 200 ns after the end of the excitation pulse. A Kaiser-Bessel window function ($\alpha = 8$) is applied and fast Fourier transformed (FFT) to obtain the spectrum in the frequency domain. The LO-2 frequency is then subtracted (for segments 1, 3, 6 and 7) or added (for segments 2, 4, 5, 8, 9 and 10) to reconstruct the molecular frequency axis, and the segments are concatenated. To account for the spurious signal generated by electronics, a background spectrum is recorded by turning off CH1 of the AWG, and the resulting spectrum is subtracted from the data spectrum. Further information on spurious signals can be found in Section S2.5.

### S1.5 Sample Chamber

The sample chamber is a CF-300 6-way cross chamber with ISO-KF-250 extensions to account for the horn antennae, and it achieves vacuum through molecular turbo pumps (HiPace 2300U and 1200 Pfeiffer), backed by a booster pump (Leybold RUVAC WSU 251) and a mechanical pump (Adixen ACP40). A working pressure of $10^{-5}$ mbar is typically achieved. The pulsed nozzle is operated at 10 Hz with an opening time $> 450$ $\mu$s. The long opening time allows for the incorporation of three pulse trains for each molecular pulse (multi-train operation), thereby making the effective repetition rate 30 Hz. The repetition rate of the instrument is mainly limited by the pumping speed, as the digitizer card allows for real time averaging. The sample is introduced into the chamber by using a pulsed valve (Parker General Valve, Series 9), which is positioned perpendicular to the axis of microwave propagation, and it is equipped with a heatable reservoir for liquid and solid samples.

### S1.6 Automation

The instrument is controlled by home-built scripts written in Python 3.5, and the software packages available for the Valon synthesizer, and for the Keysight digitizer card. The generation of the 2 GHz pulse by the Valon is controlled by its software, and the data acquisition and averaging are controlled by the Keysight soft front panel. Various steps involving adding more than 500 000 averages and FFTing the time domain, adding the LO-2 frequencies to each FID segment, stitching the spectrum together, and subtracting the background signal are controlled by a combination of scripts written in Python. After data acquisition, the complete workup process takes approximately less than 1 minute.

## S2 Results and Discussion

As coherent averaging is one of the key cornerstones of CP-FTMWs, it is important to ensure that any new design, especially one that contains several mixing and multiplication steps, retains the phase stability, dynamic range, and frequency accuracy performance associated with these instruments. While this was quickly summarized in the main text with hexanal, more details for the work presented in the main manuscript as well as measurements acquired for OCS are presented here. OCS is a linear top that has been well characterized by microwave spectroscopy in a plethora of frequency ranges. The simplicity of its spectrum, as well as its large dipole moment, has allowed for the detection of its exotic isotopologues in natural abundance, and it is an ideal molecule to demonstrate the sensitivity of microwave spectrometers.

### S2.1 Phase stability

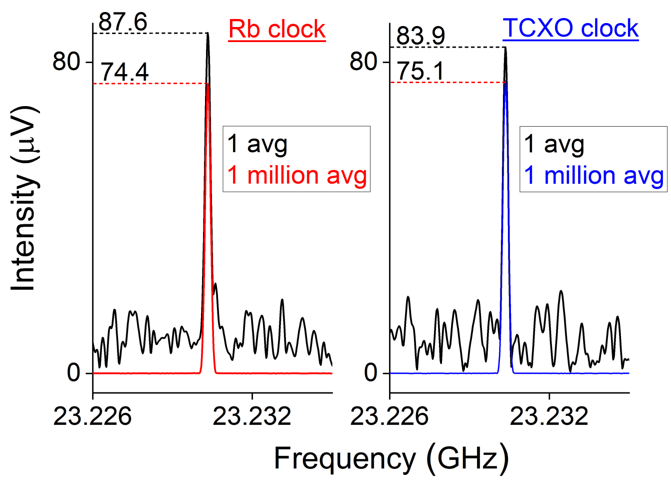


Fig. S2 A comparison between the standard rubidium clock (Rb) and the TCXO clock offered by the Valon synthesizer used as references for the 18-26 GHz instrument. Both the spectra compare the signal level for one versus one million acquisition(s) for a rotational transition of conformer 1 of hexanal.

The sensitivity that FTMW spectrometers are known for hinges on the phase stability of the instrument. This sensitivity comes from the ability to coherently average the FID signal in the time domain over many spectral acquisitions. For this, phase reproducible excitation pulses are required, and they are achieved by locking the independent components of the instrument to a low phase noise reference clock. Generally, in CP-FTMW spectrometers, a standard 10 MHz rubidium (Rb) oscillator is used[3–7]. However, as one of the aims of the design of the instrument is to reduce the cost and make the technique more attainable, alternative reference sources were considered. The Valon synthesizer, which was already integrated in the instrument's design, contains an internal temperature compensated crystal oscillator (TCXO), and thus, was a likely candidate to replace the standard Rb clock. The phase noise offered by the Rb clock is < -120 dBc/Hz, and the TCXO clock offers a phase noise of < -90 dBc/Hz, both at 10 MHz. The phase stability of the spectrometer has been evaluated using both the rubidium (Rb) and the TCXO clocks as references and the signal of transitions from hexanal. To perform the experiment with hexanal for evaluating the phase stability, the reference of the instrument was changed from the 10 MHz Rb oscillator to the TCXO clock. In both cases, the input for the clock distribution board was attached to either an output of the Rb clock or the clock output of the Valon synthesizer. In the case where the Rb clock was used, the Valon synthesizer was referenced to the Rb clock through an output of the clock distribution board (the clock output of the Valon can also be set to accept an external reference). Fig. S2 shows a comparison of the signal level of a transition of conformer 1 of hexanal taken with one average and one million averages, using a standard Rb clock or the TCXO clock offered by the Valon synthesizer as references. In both cases, the signal intensity decreases upon long averaging is approximately 10%, and this trend holds true for the rest of the spectrum. In the following section, the dynamic range of OCS is demonstrated, thereby further exhibiting the phase stability of the instrument.

### S2.2 Dynamic range

As mentioned in the main manuscript, the SNR of each conformer of hexanal can be compared between spectra obtained from UVA 18-26 GHz CP-FTMW spectromer and the Hamburg segmented 18-26 GHz CP-FTMW spectrometer, to benchmark the sensitivity of the spectrometer. Seifert et al.[5] obtained an effective SNR (after scaling) of ca. 1666:1 for conformers 1 and 2, and ca. 100:1 for conformers 3 and 4, while for the presented instrument, conformer 1 and 2 had a SNR of approximately 2330:1 and 3900:1, respectively, and conformers 3 and 4 had a SNR greater than 100:1. Fig. S3 shows the assignment of the 12 conformers of hexanal observed in the spectrum obtained from the Hamburg 18-26 GHz spectrometer.

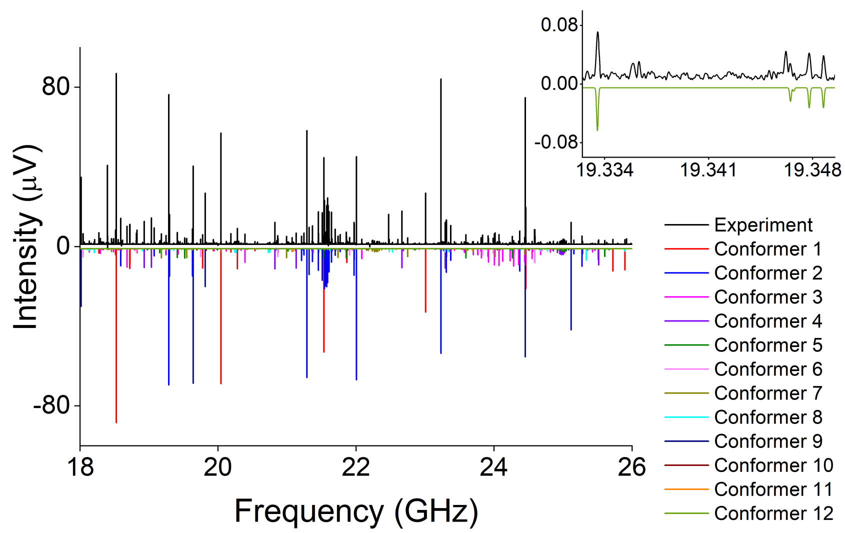


Fig. S3 The rotational spectrum of 1-hexanal measured with the segmented CP-FTMW 18-26 GHz spectrometer. The black trace shows the experimental spectrum, and the simulations of all of the 12 assigned conformers based on the experimental rotational parameters are shown in color. Inset: Zoom in of the spectrum to show conformer 12, where the labelling of the x and y axes are the same as the main figure.

Another example that demonstrates the dynamic range of the instrument is presented using OCS. A 0.2% OCS in neon mixture was supersonically expanded in the vacuum chamber using one nozzle, with 3 bar backing pressure. A total of 200 000 averages were collected and FFT'ed. Fig. S4 shows the spectrum of OCS, where the strongest transition belongs to the J = 2←1 transition of the parent species, $^{16}O^{12}C^{32}S$. The $^{18}O^{13}C^{32}S$ isotopologue, which has a natural abundance of 0.00211%, is shown in the inset of the figure. The SNR obtained for the parent species transition is approximately 100 000:1.

In the Ph.D. thesis of Dr. Daniel P. Zaleski[8], the $^{18}O^{13}C^{32}S$ isotopologue was also observed in the 18-26.5 GHz spectrometer at the University of Virginia, in a spectrum consisting of 200 000 averages. Upon scaling the SNR of the parent to account for the use of three nozzles in their experiment, they obtained an SNR of 90 000. With these results and the results from hexanal in mind, we can be confident that we do not lose sensitivity of the instrument with this new design.

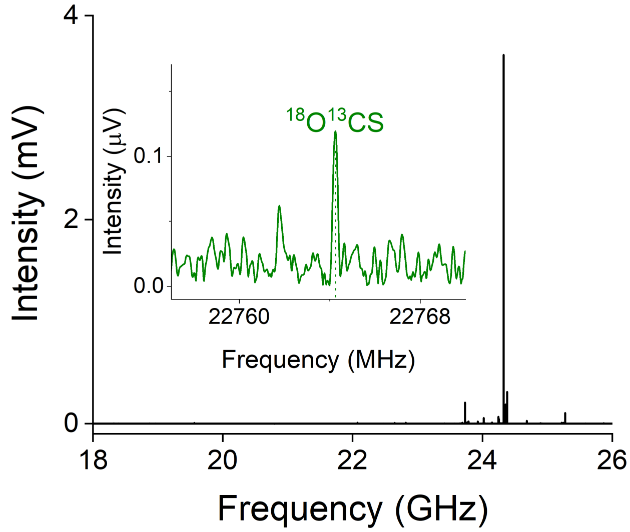


Fig. S4 The spectrum for the J=2←1 rotational transition (at 24325.9453 MHz) of OCS (0.2% in neon, 200 000 avgs). The inset shows a zoom-in on the $^{18}O^{13}C^{32}S$ isotopologue which has a natural abundance of 0.00211% (44 000 times less abundant than the normal species).

### S2.3 Intensity profile

Each of the electronic components within the circuit has a power dependence based on the frequency. This can cause intensity fluctuations across the spectrum. In order to visualize these fluctuations, a comparison of the hexanal spectra recorded in Hamburg (black trace showing 1.9 million averages) and at UVA (red trace) are shown in Fig. S5. The strongest line from the UVA spectrum (found at 23008.3685 MHz) has been scaled to the same intensity found in the Hamburg spectrum for a fair comparison. The overall intensity profile of the Hamburg spectrum follows that of the UVA spectrum[5]; however, there is a sharp intensity cut-off around 25 GHz. This is due to the aforementioned power fluctuations of the electronics. It can be seen that the excitation pulse power between 25-26 GHz is weaker compared to the 18-25 GHz range, highlighted with a blue box in Fig. S5. This will be corrected in the future by performing intensity calibrations for each segment by measuring the power response of the SSA across the whole band and applying a rectification.

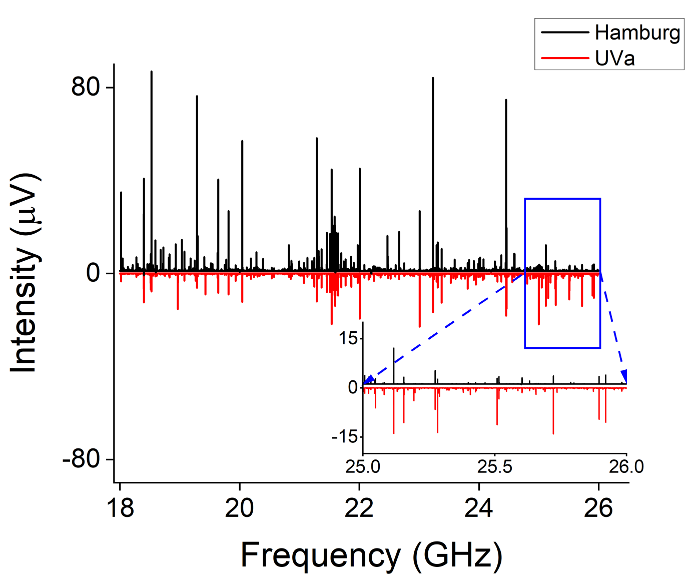


Fig. S5 Comparison of the 1-hexanal spectrum recorded in Hamburg (black trace) with the UVA spectrum previously reported (red trace). The blue box highlights the sharp cutoff in the intensity >25 GHz (see text for more detail). Inset: Zoom in of the spectrum to show the intensity comparison in the highlighted box, where the labelling of the x and y axes are the same as the main figure.

### S2.4 Frequency accuracy and resolution

Microwave spectroscopy is known to provide precise transition frequencies of a molecule. These frequencies should be the same (within the experimental error of the instrument) between spectrometers. If this is not the case, it speaks of frequency jitter that could be present in some of the electronics being used within the circuit. Thus, it is important to characterize the frequency accuracy of the instrument.

As mentioned in the main manuscript, the frequency accuracy of the instrument has been benchmarked by comparing the center frequencies determined for all of the measured rotational transitions of conformer 1 of hexanal and its $^{18}$O isotopologue obtained from the UVA 18-26 GHz CP-FTMW spectrometer[5] to those obtained from the segmented 18-26 GHz CP-FTMW spectrometer, and this is further elaborated here. For simplicity in the following discussion, the UVA 18-26 GHz CP-FTMW spectrometer is referred to as 'UVA', and the segmented 18-26 GHz CP-FTMW spectrometer as 'Hamburg'. The measured transitions of conformer 1 of hexanal and its $^{18}$O isotopologue obtained from the UVA spectrometer were fit to an asymmetric rotational Hamiltonian to generate a set of rotational constants for each species. Along with these rotational constants, root mean square (RMS) errors, which tallies the observed minus calculated (OMC) values for the transition frequencies, were obtained. From the assigned rotational transitions with the UVA spectrometer, an RMS value of ∼4 kHz and ∼7 kHz was obtained for conformer 1 of hexanal and its $^{18}$O isotopologue, respectively. The fitting procedure was done for the assigned transitions from the Hamburg spectrometer, in which the rotational constants were fixed to the values that were found from the UVA spectrometer. RMS values of ∼12.7 kHz for conformer 1 and ∼17 kHz for the $^{18}$O isotopologue are obtained. In this case, the individual OMC values were observed to be less than 20 kHz, except for one discrepancy. The measured transitions from the Hamburg spectrometer were also fit to an asymmetric rotational Hamiltonian where the rotational constants were allowed to be fit. This resulted in RMS values of ∼6 kHz for conformer 1 of hexanal and ∼9 kHz for its $^{18}$O isotopologue. Here, the difference between the OMC values is below 10 kHz, for both species. A summary of the fits is given in Table S1, and their corresponding transitions are given in Tables S7-S8 of the Supplementary Material. The deviation in the A, B, and C rotational constants from the Hamburg spectrometer compared to those from the UVA spectrometer is less than 0.001% in both cases. The RMS values of the Hamburg spectrometer closely match those of the UVA spectrometer.

Table S1 A comparison of the rotational constants (A, B, C) and distortion constants ($\Delta_J$, $\Delta_{JK}$, $\Delta_K$, $\delta_J$) for conformer 1 of hexanal and its $^{18}$O isotopologue, obtained from the UVA CP-FTMW spectrometer, as presented in Reference[5], and the Hamburg segmented CP-FTMW spectrometer, as presented in this work.

| | Conformer 1 | | | $^{18}$O Conformer 1 | | |
|---|---|---|---|---|---|---|
| | UVA[5] | Hamburg | | UVA[5] | Hamburg | |
| | | Fixed[a] | Floated | | Fixed[b] | Floated[c] |
| A (MHz) | 9769.6385(41) | [9769.6385] | 9769.6429(61) | 9511.5910(64) | [9511.5910] | 9511.6030(87) |
| B (MHz) | 868.84583(21) | [868.84583] | 868.84861(32) | 843.5515(31) | [843.5515] | 843.5600(42) |
| C (MHz) | 818.51887(19) | [818.51887] | 818.52102(28) | 794.2703(11) | [794.2703] | 794.2745(15) |
| $\Delta_J$ (kHz) | 0.04597(48) | [0.04597] | 0.05281(72) | [0.04597] | [0.04597] | [0.05281] |
| $\Delta_{JK}$ (kHz) | −0.8782(47) | [-0.8782] | −0.8497(70) | [−0.8782] | [-0.8782] | [−0.8497] |
| $\Delta_K$ (kHz) | 25.70(79) | [25.70] | 24.5(11) | [25.70] | [25.70] | [24.5] |
| $\delta_J$ (kHz) | 0.00514(18) | [0.00514] | 0.00530(27) | [0.00514] | [0.00514] | [0.00530] |
| Number of lines | 46 | 46 | 46 | 6 | 6 | 6 |
| $\sigma$ (kHz) | 4.1 | 12.7 | 6.0 | 6.7 | 17.0 | 9.0 |

[a] fixed to the assignments from the UVA CP-FTMW spectrometer for the conformer 1 of hexanal.
[b] fixed to the assignments from the UVA CP-FTMW spectrometer for the $^{18}$O isotopologue of conformer 1 of hexanal.
[c] fixed to the assignments from the floated values for the Hamburg CP-FTMW spectrometer for the conformer 1 of hexanal.

Another example that demonstrates the frequency accuracy is presented using OCS. Table S2 shows a comparison of the frequencies measured with the segmented CP-FTMW spectrometer and the experimental values from the literature. The agreement between the segmented CP-FTMW frequencies and the literature frequencies are of the order of 20 kHz, and its deviation is less than 0.1%. This, combined with the fact that similar RMS values were obtained for hexanal between the two instruments, indicates that this design is a viable alternative to the direct excitation and detection design.

Table S2 Comparison of the J=2←1 rotational transition of OCS obtained with the segmented CP-FTMW spectrometer with reported values in the literature.

| Isotopologue | F'←F | Segmented CP-FTMW freq. (MHz) | Lit. freq. (MHz) | Difference (kHz) | Percentage difference (%) |
|---|---|---|---|---|---|
| OCS | | 24325.9453 | 24325.930(10)[a] | 15.3 | 0.06 |
| $OC^{34}S$ | | 23731.3112 | 23731.302(10)[a] | 9.2 | 0.04 |
| $O^{13}CS$ | | 24247.6799 | 24247.668(10)[a] | 11.9 | 0.05 |
| $OC^{33}S$ | | | | | |
| | 3/2-1/2 | 24012.3693 | 24012.345(5)[b] | 24.3 | 0.10 |
| | 5/2-5/2 | 24012.9908 | 24012.964(5)[b] | 26.8 | 0.11 |
| | 5/2-3/2 | | 24020.249(5)[b,+] | | |
| | 7/2-5/2 | 24020.2733 | 24020.249(5)[b,+] | 24.3 | 0.10 |
| | 3/2-3/2 | 24025.4709 | 24025.488(5)[b] | 22.9 | 0.10 |
| $^{18}OCS$ | | 22819.4130 | 22819.3930(10)[c] | 20.0 | 0.09 |
| $O^{13}C^{34}S$ | | 23646.9155 | 23646.8935(10)[c] | 22.0 | 0.09 |
| $^{17}OCS$ | 9/2-7/2 | 23534.6933 | 23534.6780(5)[b] | 15.3 | 0.07 |
| $OC^{36}S$ | | 23198.7541 | 23198.7344(10)[c] | 19.7 | 0.08 |
| $^{18}OC^{34}S$ | | 22239.8590 | 22239.8438(10)[c] | 15.2 | 0.07 |
| $O^{13}C^{33}S$ | | 23938.8379 | 23938.8340(21)[d] | 3.9 | 0.02 |
| $^{18}O^{13}CS$ | | 22764.2483 | 22764.240(20)[e] | 8.3 | 0.04 |

[a] Bomsdorf, H., Dreizler, H. & Mäder, H. (1980). Zeitschrift für Naturforschung A, 35(7), pp. 723-730.
[b] Merke, I. & Dreizler, H. (1987). Zeitschrift für Naturforschung A, 42(9), pp. 1043-1044.
[c] R. D. Suenram, private communications (1998).
[d] F. J. Lovas, J. Phys. Chem., 7, (1978), 1445-1750.
[e] H. S. P. Müller, F. Schlöder, J. Stutzki, and G. Winnewisser, J. Mol. Struct. 742, (2005), 215-227.
[+] For $OC^{33}S$, the F=5/2-3/2 and the 7/2-5/2 transitions are blended at the experiment resolution.

### S2.5 Electronic response

The spectra from CP-FTMW spectrometers are quite congested, with rotational transitions from multiple conformers, isomers, complexes, and isotopologues present. Due to the high density of lines, signals arising from the electrical responses of the circuit's components, or spurious signals, are unwanted and only serve to make identifying weak species within the spectrum more difficult. In addition, they can also mix with molecular signals leading to false intensity patterns. Their presence in CP-FTMW spectrometers has been previously reported[6], thus we investigated their presence within this design. The fact that this instrument requires several mixing stages can enhance their manifestation, especially if high fidelity AWGs are not used. While a high fidelity AWG has been used in the 18-26 GHz spectrometer, there are strong spurious signals every 200 MHz while looking at the background spectrum and some weak spurs in between. To remove them, the electronic response spectrum of the spectrometer taken at the same number of acquisitions as the molecular spectrum is subtracted from the molecular spectrum. As the intensity fluctuation of the spurs is random, the subtraction process does not guarantee removal of all the spurs, and it can sometimes result in negative "intensities" in the final spectrum. This method also does not remove spurs that come from the mixing of spurious signals with molecular signals. Fig. S6 shows a comparison of sections of the hexanal spectrum recorded in Hamburg (black trace) and the UVA spectrum previously reported (red trace). This highlights the fact that there are still spurious signals seen in the Hamburg spectrum. Further work needs to be conducted on how best to reduce their influence on the spectrum.

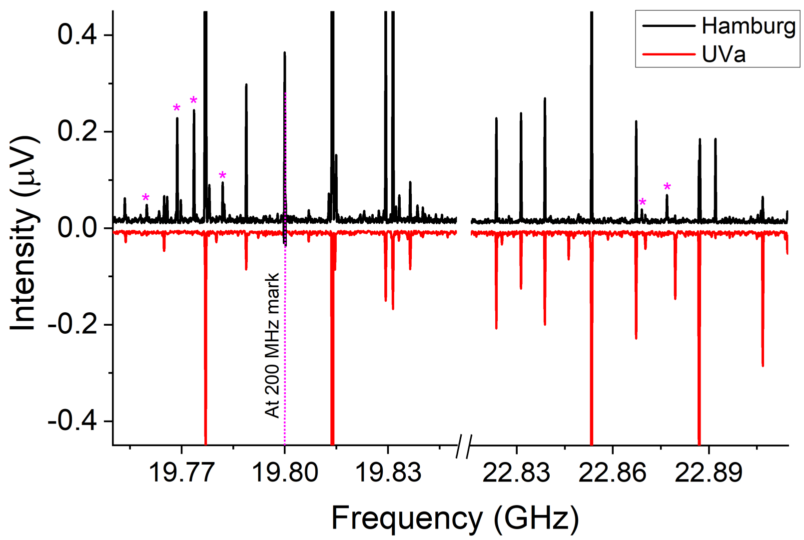


Fig. S6 Comparison of the hexanal spectrum recorded in Hamburg (top black trace) with the UVA spectrum previously reported (bottom red trace). The spurious signals are highlighted with asterisks.

## S3 Conclusion

The work presented here successfully demonstrates the design and performance of a K-band segmented chirped-pulse FTMW instrument. The principle design of the spectrometer is based on the segmented chirped-pulse approach and multi-train method in order to reduce the cost of building a CP-FTMW spectrometer without sacrificing the performance or broadband capabilities. Table S3 shows a cost comparison of this design to the previously reported broadband CP-FTMW instrument. By replacing the expensive traveling wave tube amplifier (TWTA) with a solid-state amplifier (SSA), the standard 10 MHz rubidium (Rb) oscillator with an internal temperature compensated crystal oscillator (TCXO) clock of the Valon synthesizer, and the oscilloscope with a high-speed, PCIe digitizer card, it is possible to decrease the cost of the instrument by a factor of at least two, without compromising on the instrument's performance (based on the dynamic range and the frequency accuracy of the instrument). The instrument offers another significant advantage over the broadband designs, as the oscilloscopes used typically have high data transfer rates. This limits the effective repetition rate to less than 100 Hz. With the proper vacuum setup, this instrument could achieve real time data acquisition rates with minimal data transfer times, thus decreasing spectral acquisition times from a few days (in the case of 1,000,000 acquisition spectra or larger) to hours. Work still needs to be done to optimize the removal of spurious signals, as well as optimize the intensity calibration. This instrument has the capability to incorporate electric discharge and laser ablation techniques to study unstable species or molecules with low vapor pressure, which will widen even further the scope of its applicability to astrochemical studies.

Table S3 An approximate cost comparison of the single chirp 18-26 GHz CP-FTMW spectrometer at UVA [5] with the segmented 18-26 GHz CP-FTMW spectrometer built and characterized in this thesis.

| | CP-FTMW | Segmented CP-FTMW |
|---|---|---|
| Effective Rep. Rate | 30 Hz | 30 Hz |
| Power/GHz | 5 W/GHz | 6 W/GHz |
| Bandwidth | 8 GHz/segment | 800 MHz/segment |
| Number of nozzles | 3 | 1 |
| FID Duration | 10 $\mu$s | 10 $\mu$s |
| LNA | 48 dB | 45 dB |
| Cost | ~ €350,000 | ~ €150,000 |
| SNR of $^{18}O^{12}C^{32}S$ (200 000 averages) | 90 000:1 [a] | 100 000:1 |

[a] *scaled for one nozzle.*

## S4 Fitted rotational constants for the isotopologues of Conformers I, II and III of isoleucinol

Table S4 Experimental rotational constants of $^{13}C$, $^{18}O$ and $^{15}N$ for Conformer I of isoleucinol. Quartic centrifugal distortion constants ($\Delta_J$, $\Delta_{JK}$) and nitrogen quadruple parameters ($\chi_{aa}$, $\chi_{bb}$ - $\chi_{cc}$) are kept fixed to the parent species.

| | Parent | $^{13}$C1 | $^{13}$C2 | $^{13}$C3 | $^{13}$C4 |
|---|---|---|---|---|---|
| A (MHz) | 3759.34376(39) | 3745.439(35) | 3756.411(35) | 3756.186(34) | 3745.884(32) |
| B (MHz) | 1062.44909(12) | 1055.21888(38) | 1061.45345(44) | 1061.18462(53) | 1054.47780(44) |
| C (MHz) | 880.24579(13) | 874.74707(33) | 879.60403(39) | 879.34464(39) | 874.51694(34) |
| $\Delta_J$ (kHz) | 0.02663(55) | [0.02663] | [0.02663] | [0.02663] | [0.02663] |
| $\Delta_{JK}$ (kHz) | 0.3348(82) | [0.3348] | [0.3348] | [0.3348] | [0.3348] |
| $\chi_{aa}$*1.5 (MHz) | −6.3228(46) | [−6.3228] | [−6.3228] | [−6.3228] | [−6.3228] |
| ($\chi_{bb}$ - $\chi_{cc}$)*0.25 (MHz) | 0.1242(15) | [0.1242] | [0.1242] | [0.1242] | [0.1242] |
| Number of lines | 357 | 34 | 33 | 32 | 27 |
| $\sigma$ (kHz) | 12.5 | 8.7 | 11 | 12.2 | 9.2 |

| | $^{13}$C5 | $^{13}$C6 | $^{18}$O | $^{15}$N |
|---|---|---|---|---|
| A (MHz) | 3755.137(58) | 3674.659(34) | [3757.59259] | 3690.030(54) |
| B (MHz) | 1039.47661(63) | 1060.41821(49) | 1023.07060(96) | 1060.34811(97) |
| C (MHz) | 864.32850(47) | 874.16456(37) | 853.03472(75) | 875.01893(65) |
| $\Delta_J$ (kHz) | [0.02663] | [0.02663] | [0.02663] | [0.02663] |
| $\Delta_{JK}$ (kHz) | [0.3348] | [0.3348] | [0.3348] | [0.3348] |
| $\chi_{aa}$*1.5 (MHz) | [−6.3228] | [−6.3228] | [−6.3228] | – |
| ($\chi_{bb}$ - $\chi_{cc}$)*0.25 (MHz) | [0.1242] | [0.1242] | [0.1242] | – |
| Number of lines | 32 | 33 | 4 | 14 |
| $\sigma$ (kHz) | 14.7 | 10.7 | 4.3 | 11.6 |

Table S5 Experimental rotational constants of $^{13}C$ for Conformer II of isoleucinol. Quartic centrifugal distortion constants ($\Delta_J$, $\Delta_{JK}$, $\delta_J$) and nitrogen quadruple parameters ($\chi_{aa}$, $\chi_{bb}$ - $\chi_{cc}$) are kept fixed to the parent species.

| | Parent | $^{13}$C1 | $^{13}$C2 | $^{13}$C3 |
|---|---|---|---|---|
| A (MHz) | 3170.22321(33) | 3153.58(10) | 3165.81(10) | 3164.531(72) |
| B (MHz) | 1103.61682(17) | 1097.5552(11) | 1102.31684(92) | 1101.65514(70) |
| C (MHz) | 971.59291(15) | 965.80927(81) | 970.32954(76) | 970.44690(76) |
| $\Delta_J$ (kHz) | 0.08475(84) | [0.08475] | [0.08475] | [0.08475] |
| $\Delta_{JK}$ (kHz) | −0.3651(58) | [−0.3651(58)] | [−0.3651(58)] | [−0.3651(58)] |
| $\delta_J$ (kHz) | 0.01271(62) | [0.01271(62)] | [0.01271(62)] | [0.01271(62)] |
| $\chi_{aa}$*1.5 (MHz) | −6.3234(50) | [−6.3234(50)] | [−6.3234(50)] | [−6.3234(50)] |
| ($\chi_{bb}$ - $\chi_{cc}$)*0.25 (MHz) | −0.1286(15) | [−0.1286(15)] | [−0.1286(15)] | [−0.1286(15)] |
| Number of lines | 323 | 8 | 11 | 13 |
| $\sigma$ (kHz) | 11.4 | 8.7 | 9.6 | 11.3 |

| | $^{13}$C4 | $^{13}$C5 | $^{13}$C6 |
|---|---|---|---|
| A (MHz) | 3155.143(53) | 3146.571(91) | 3115.826(77) |
| B (MHz) | 1097.81391(52) | 1083.9272(11) | 1097.4694(10) |
| C (MHz) | 966.74006(42) | 954.15626(77) | 962.94059(72) |
| $\Delta_J$ (kHz) | [0.08475] | [0.08475] | [0.08475] |
| $\Delta_{JK}$ (kHz) | [−0.3651(58)] | [−0.3651(58)] | [−0.3651(58)] |
| $\delta_J$ (kHz) | [0.01271(62)] | [0.01271(62)] | [0.01271(62)] |
| $\chi_{aa}$*1.5 (MHz) | [−6.3234(50)] | [−6.3234(50)] | [−6.3234(50)] |
| ($\chi_{bb}$ - $\chi_{cc}$)*0.25 (MHz) | [−0.1286(15)] | [−0.1286(15)] | [−0.1286(15)] |
| Number of lines | 14 | 7 | 12 |
| $\sigma$ (kHz) | 6.4 | 6.0 | 7.9 |

Table S6 Experimental rotational constants of $^{13}$C for Conformer III of isoleucinol. Quartic centrifugal distortion constants ($\Delta_J$, $\Delta_{JK}$, $\delta_J$) and nitrogen quadruple parameters ($\chi_{aa}$, $\chi_{bb}$ - $\chi_{cc}$) are kept fixed to the parent species.

| | Parent | $^{13}$C1 | $^{13}$C2 | $^{13}$C3 |
|---|---|---|---|---|
| A (MHz) | 3067.56626(32) | 3059.714(46) | 3066.875(42) | 3057.472(54) |
| B (MHz) | 1213.42566(16) | 1204.58462(74) | 1212.83793(87) | 1210.9503(15) |
| C (MHz) | 1010.54858(14) | 1003.61816(78) | 1010.09609(73) | 1009.01817(61) |
| $\Delta_J$ (kHz) | 0.11429(88) | [0.11429] | [0.11429] | [0.11429] |
| $\Delta_{JK}$ (kHz) | −0.2067(55) | [−0.2067] | [−0.2067] | [−0.2067] |
| $\delta_J$ (kHz) | 0.02256(63) | [0.02256] | [0.02256] | [0.02256] |
| $\chi_{aa}$*1.5 (MHz) | −5.2345(49) | [−5.2345] | [−5.2345] | [−5.2345] |
| ($\chi_{bb}$ - $\chi_{cc}$)*0.25 (MHz) | 0.1195(15) | [0.1195] | [0.1195] | [0.1195] |
| Number of lines | 269 | 18 | 16 | 16 |
| $\sigma$ (kHz) | 11.2 | 11.5 | 12.1 | 13.2 |

| | $^{13}$C4 | $^{13}$C5 | $^{13}$C6 |
|---|---|---|---|
| A (MHz) | 3060.334(65) | 3043.051(47) | 3003.892(31) |
| B (MHz) | 1201.14812(99) | 1193.35906(83) | 1210.46269(79) |
| C (MHz) | 1002.20154(79) | 997.17711(60) | 1001.52083(49) |
| $\Delta_J$ (kHz) | [0.11429] | [0.11429] | [0.11429] |
| $\Delta_{JK}$ (kHz) | [−0.2067] | [−0.2067] | [−0.2067] |
| $\delta_J$ (kHz) | [0.02256] | [0.02256] | [0.02256] |
| $\chi_{aa}$*1.5 (MHz) | [−5.2345] | [−5.2345] | [−5.2345] |
| ($\chi_{bb}$ - $\chi_{cc}$)*0.25 (MHz) | [0.1195] | [0.1195] | [0.1195] |
| Number of lines | 14 | 15 | 14 |
| $\sigma$ (kHz) | 10.7 | 9.9 | 11.8 |

## S5 Linelist for the conformer 1 of hexanal and its $^{18}$O isotopologue

Table S7 Linelist for conformer 1 of hexanal. OMC is the difference between the observed and calculated transition. The frequency accuracy to fit the transitions was set to 20 kHz. Fixed OMCs correspond to the difference between the calculated transitions from the UVA fitted rotational parameters and the observed transitions from the Hamburg spectrometer. Floated OMCs correspond to the difference between the calculated transitions from the Hamburg fitted rotational parameters and the observed transitions from the Hamburg spectrometer.

| $J'$ | $K_{a'}$ | $K_{c'}$ | | $J$ | $K_a$ | $K_c$ | Observed (MHz) | OMC (MHz) Fixed | OMC (MHz) Floated |
|---|---|---|---|---|---|---|---|---|---|
| 11 | 1 | 11 | ← | 10 | 1 | 10 | 18272.9760 | 0.0130 | -0.0012 |
| 11 | 0 | 11 | ← | 10 | 0 | 10 | 18514.2640 | 0.0132 | -0.0036 |
| 6 | 1 | 6 | ← | 5 | 0 | 5 | 18525.9833 | 0.0130 | -0.0062 |
| 11 | 2 | 10 | ← | 10 | 2 | 9 | 18553.5751 | 0.0113 | -0.0037 |
| 11 | 5 | 7 | ← | 10 | 5 | 6 | 18563.6154 | 0.0086 | 0.0065 |
| 11 | 4 | 8 | ← | 10 | 4 | 7 | 18564.6171 | 0.0060 | -0.0017 |
| 11 | 3 | 9 | ← | 10 | 3 | 8 | 18566.8922 | 0.0194 | 0.0072 |
| 11 | 3 | 8 | ← | 10 | 3 | 7 | 18567.5916 | -0.0041 | -0.0164 |
| 15 | 0 | 15 | ← | 14 | 1 | 14 | 18616.0808 | 0.0084 | 0.0054 |
| 4 | 2 | 2 | ← | 5 | 1 | 5 | 18722.6930 | 0.0109 | 0.0051 |
| 11 | 1 | 10 | ← | 10 | 1 | 9 | 18825.7949 | 0.0133 | -0.0062 |
| 12 | 1 | 12 | ← | 11 | 1 | 11 | 19931.8250 | 0.0100 | 0.0019 |
| 7 | 1 | 7 | ← | 6 | 0 | 6 | 20041.8871 | 0.0142 | -0.0041 |
| 12 | 0 | 12 | ← | 11 | 0 | 11 | 20187.7581 | 0.0107 | 0.0001 |
| 12 | 2 | 11 | ← | 11 | 2 | 10 | 20238.5833 | 0.0124 | 0.0035 |
| 12 | 5 | 7 | ← | 11 | 5 | 6 | 20251.5656 | 0.0012 | 0.0064 |
| 12 | 4 | 9 | ← | 11 | 4 | 8 | 20252.9098 | 0.0066 | 0.0056 |
| 12 | 3 | 10 | ← | 11 | 3 | 9 | 20255.7929 | 0.0155 | 0.0097 |
| 12 | 3 | 9 | ← | 11 | 3 | 8 | 20256.9055 | 0.0037 | -0.0020 |
| 12 | 2 | 10 | ← | 11 | 2 | 9 | 20298.8864 | 0.0120 | 0.0019 |
| 12 | 1 | 11 | ← | 11 | 1 | 10 | 20534.5539 | 0.0109 | -0.0026 |
| 16 | 0 | 16 | ← | 15 | 1 | 15 | 20567.6169 | -0.0126 | -0.0026 |
| 8 | 1 | 8 | ← | 7 | 0 | 7 | 21535.6561 | 0.0138 | -0.0023 |
| 13 | 1 | 13 | ← | 12 | 1 | 12 | 21590.0992 | 0.0039 | 0.0037 |
| 13 | 0 | 13 | ← | 12 | 0 | 12 | 21858.8462 | 0.0111 | 0.0086 |
| 13 | 2 | 12 | ← | 12 | 2 | 11 | 21923.1390 | -0.0014 | -0.0021 |
| 13 | 4 | 10 | ← | 12 | 4 | 9 | 21941.3323 | -0.0187 | -0.0109 |
| 13 | 3 | 11 | ← | 12 | 3 | 10 | 21944.9123 | 0.0026 | 0.0052 |
| 13 | 3 | 10 | ← | 12 | 3 | 9 | 21946.5817 | -0.0134 | -0.0109 |
| 13 | 2 | 11 | ← | 12 | 2 | 10 | 21999.6310 | 0.0026 | 0.0004 |
| 13 | 1 | 12 | ← | 12 | 1 | 11 | 22242.5747 | 0.0049 | -0.0006 |
| 17 | 0 | 17 | ← | 16 | 1 | 16 | 22523.0901 | -0.0274 | -0.0014 |
| 9 | 1 | 9 | ← | 8 | 0 | 8 | 23008.3685 | 0.0142 | 0.0016 |
| 14 | 1 | 14 | ← | 13 | 1 | 13 | 23247.7630 | -0.0077 | 0.0022 |
| 14 | 0 | 14 | ← | 13 | 0 | 13 | 23527.3723 | -0.0017 | 0.0060 |
| 15 | 2 | 13 | ← | 15 | 1 | 14 | 24308.8210 | -0.0168 | -0.0015 |
| 10 | 1 | 10 | ← | 9 | 0 | 9 | 24461.2573 | 0.0131 | 0.0058 |
| 13 | 2 | 11 | ← | 13 | 1 | 12 | 24804.8827 | -0.0233 | -0.0142 |
| 15 | 1 | 15 | ← | 14 | 1 | 14 | 24904.7836 | -0.0275 | -0.0051 |
| 12 | 2 | 10 | ← | 12 | 1 | 11 | 25047.8543 | 0.0068 | 0.0125 |
| 15 | 0 | 15 | ← | 14 | 0 | 14 | 25193.2218 | -0.0262 | -0.0058 |
| 11 | 2 | 9 | ← | 11 | 1 | 10 | 25283.5124 | -0.0037 | -0.0014 |
| 10 | 2 | 8 | ← | 10 | 1 | 9 | 25509.2206 | -0.0014 | -0.0026 |
| 9 | 2 | 7 | ← | 9 | 1 | 8 | 25722.4758 | 0.0058 | 0.0011 |
| 11 | 1 | 11 | ← | 10 | 0 | 10 | 25895.7089 | 0.0069 | 0.0065 |
| 8 | 2 | 6 | ← | 8 | 1 | 7 | 25920.9812 | 0.0090 | 0.0010 |
| | | | | | | | RMS | 12.7 kHz | 6.0 kHz |

Table S8 Linelist for $^{18}O$ isotopologue of conformer 1 of hexanal. OMC is the difference between the observed and calculated transition. The frequency accuracy to fit the transitions was set to 20 kHz. Fixed OMCs correspond to the difference between the calculated transitions from the UVA fitted rotational parameters and the observed transitions from the Hamburg spectrometer. Floated OMCs correspond to the difference between the calculated transitions from the Hamburg fitted rotational parameters and the observed transitions from the Hamburg spectrometer.

| J' | $K_{a'}$ | $K_{c'}$ | | J | $K_a$ | $K_c$ | Observed (MHz) | OMC (MHz) Fixed | OMC (MHz) Fitted |
|---|---|---|---|---|---|---|---|---|---|
| 7 | 1 | 7 | ← | 6 | 0 | 6 | 19476.3309 | 0.0313 | 0.0046 |
| 8 | 1 | 8 | ← | 7 | 0 | 7 | 20924.6072 | 0.0167 | -0.002 |
| 9 | 1 | 9 | ← | 8 | 0 | 8 | 22352.2767 | -0.0070 | -0.0153 |
| 10 | 1 | 10 | ← | 9 | 0 | 9 | 23760.6029 | 0.0073 | 0.0122 |
| 5 | 2 | 3 | ← | 5 | 1 | 4 | 25716.3034 | -0.0041 | -0.0061 |
| 4 | 2 | 2 | ← | 4 | 1 | 3 | 25834.8541 | 0.0189 | 0.0063 |
| | | | | | | | | 17.0 kHz | 9.0 kHz |

## S6 Linelist for the conformers of isoleucinol

In the following lines lists belonging to the fits for Conformers I-VII, for the 2-8 GHz the frequency accuracy for the transitions were set to 15 kHz. As the nuclear quadrupole coupling decreases with increasing *J*, the hyperfine splitting starts merging in the 8-26 GHz region. This results in broadening of the linewidth in the spectra. In order to account for this fact, the frequency accuracy for the fits in the 8-18 GHz and 18-26 GHz were set to 25kHz and 30 kHz, respectively, instead of 20 kHz.

Table S9 Linelist for Conformer I of isoleucinol. OMC is the difference between the observed and calculated transition.

| J' | $K_{a'}$ | $K_{c'}$ | F' | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 1 | 2 | 3 | ← | 2 | 0 | 2 | 3 | 2523.4584 | 0.0122 |
| 5 | 1 | 4 | 5 | ← | 4 | 2 | 2 | 4 | 2523.5540 | -0.0045 |
| 1 | 1 | 0 | 2 | ← | 1 | 0 | 1 | 2 | 2878.8012 | 0.0076 |
| 1 | 1 | 0 | 1 | ← | 1 | 0 | 1 | 2 | 2879.3565 | 0.0057 |
| 1 | 1 | 0 | 2 | ← | 1 | 0 | 1 | 1 | 2880.0664 | 0.0085 |
| 2 | 1 | 1 | 3 | ← | 2 | 0 | 2 | 3 | 3070.1024 | 0.0108 |
| 2 | 1 | 1 | 2 | ← | 2 | 0 | 2 | 2 | 3070.6930 | 0.0113 |
| 3 | 0 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 3268.3353 | -0.0065 |
| 3 | 0 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 3269.1337 | 0.0032 |
| 3 | 1 | 2 | 2 | ← | 3 | 0 | 3 | 2 | 3373.2074 | 0.0010 |
| 2 | 1 | 2 | 2 | ← | 1 | 1 | 1 | 1 | 3702.1267 | -0.0043 |
| 2 | 1 | 2 | 2 | ← | 1 | 1 | 1 | 2 | 3702.8371 | -0.0005 |
| 2 | 1 | 2 | 1 | ← | 1 | 1 | 1 | 1 | 3703.0599 | -0.0014 |
| 2 | 1 | 2 | 3 | ← | 1 | 1 | 1 | 2 | 3703.4341 | -0.0008 |
| 2 | 1 | 2 | 1 | ← | 1 | 1 | 1 | 0 | 3704.8323 | 0.0044 |
| 4 | 1 | 3 | 4 | ← | 4 | 0 | 4 | 3 | 3805.3584 | 0.0054 |
| 4 | 1 | 3 | 4 | ← | 4 | 0 | 4 | 5 | 3805.7197 | 0.0057 |
| 2 | 0 | 2 | 2 | ← | 1 | 0 | 1 | 2 | 3875.2069 | 0.0000 |
| 2 | 0 | 2 | 1 | ← | 1 | 0 | 1 | 0 | 3875.4085 | 0.0022 |
| 2 | 0 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 3876.5549 | 0.0007 |
| 2 | 0 | 2 | 1 | ← | 1 | 0 | 1 | 2 | 3877.3029 | -0.0004 |
| 2 | 0 | 2 | 1 | ← | 1 | 0 | 1 | 1 | 3878.5685 | 0.0007 |
| 2 | 1 | 1 | 2 | ← | 1 | 1 | 0 | 1 | 4066.5444 | 0.0066 |
| 2 | 1 | 1 | 2 | ← | 1 | 1 | 0 | 2 | 4067.0985 | 0.0035 |
| 2 | 1 | 1 | 3 | ← | 1 | 1 | 0 | 2 | 4067.8573 | 0.0050 |
| 2 | 1 | 1 | 1 | ← | 1 | 1 | 0 | 0 | 4069.1139 | 0.0039 |
| 4 | 0 | 4 | 3 | ← | 3 | 1 | 2 | 2 | 4309.5038 | 0.0069 |
| 5 | 1 | 4 | 5 | ← | 5 | 0 | 5 | 5 | 4392.9060 | -0.0051 |
| 1 | 1 | 1 | 0 | ← | 0 | 0 | 0 | 1 | 4638.4158 | 0.0047 |
| 1 | 1 | 1 | 2 | ← | 0 | 0 | 0 | 1 | 4639.4780 | 0.0068 |
| 1 | 1 | 1 | 1 | ← | 0 | 0 | 0 | 1 | 4640.1893 | 0.0116 |
| 1 | 1 | 0 | 0 | ← | 0 | 0 | 0 | 1 | 4820.8678 | 0.0048 |
| 1 | 1 | 0 | 2 | ← | 0 | 0 | 0 | 1 | 4821.7022 | 0.0030 |
| 1 | 1 | 0 | 1 | ← | 0 | 0 | 0 | 1 | 4822.2520 | -0.0044 |
| 4 | 0 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 5402.0912 | 0.0044 |
| 4 | 0 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 5402.5074 | -0.0133 |
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 3 | 5548.4698 | 0.0008 |
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 5549.0652 | -0.0011 |
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 5549.4380 | 0.0006 |
| 3 | 1 | 3 | 2 | ← | 2 | 1 | 2 | 1 | 5549.4380 | -0.0060 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 1 | 3 | 2 | ← | 2 | 1 | 2 | 2 | 5550.3788 | 0.0044 |
| 5 | 0 | 5 | 4 | ← | 4 | 1 | 3 | 4 | 5735.7181 | 0.0074 |
| 3 | 0 | 3 | 3 | ← | 2 | 0 | 2 | 3 | 5791.1904 | -0.0002 |
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 1 | 5792.3138 | 0.0008 |
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 5792.5666 | -0.0100 |
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 3 | 5793.0612 | -0.0009 |
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 2 | 5794.4129 | 0.0034 |
| 3 | 2 | 2 | 3 | ← | 2 | 2 | 1 | 2 | 5827.0265 | 0.0062 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 2 | 5827.0265 | 0.0058 |
| 3 | 2 | 2 | 4 | ← | 2 | 2 | 1 | 3 | 5828.3801 | 0.0051 |
| 3 | 2 | 2 | 3 | ← | 2 | 2 | 1 | 3 | 5828.3801 | 0.0050 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 3 | 5828.3801 | 0.0046 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 1 | 5829.1357 | 0.0077 |
| 3 | 2 | 1 | 3 | ← | 2 | 2 | 0 | 2 | 5862.5716 | 0.0075 |
| 3 | 2 | 1 | 4 | ← | 2 | 2 | 0 | 3 | 5863.9355 | 0.0052 |
| 3 | 2 | 1 | 2 | ← | 2 | 2 | 0 | 3 | 5863.9355 | -0.0019 |
| 3 | 2 | 1 | 2 | ← | 2 | 2 | 0 | 1 | 5864.6926 | 0.0067 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 3 | 6094.6443 | -0.0012 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 6095.4036 | 0.0007 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6095.7869 | 0.0072 |
| 3 | 1 | 2 | 2 | ← | 2 | 1 | 1 | 2 | 6096.9372 | 0.0029 |
| 2 | 1 | 2 | 1 | ← | 1 | 0 | 1 | 0 | 6398.4374 | 0.0012 |
| 2 | 1 | 2 | 2 | ← | 1 | 0 | 1 | 2 | 6399.4008 | -0.0022 |
| 2 | 1 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 6399.9990 | -0.0013 |
| 2 | 1 | 2 | 2 | ← | 1 | 0 | 1 | 1 | 6400.6671 | -0.0002 |
| 2 | 1 | 2 | 1 | ← | 1 | 0 | 1 | 1 | 6401.5990 | 0.0013 |
| 6 | 2 | 5 | 5 | ← | 6 | 1 | 5 | 5 | 6529.4248 | 0.0108 |
| 6 | 2 | 5 | 6 | ← | 6 | 1 | 5 | 6 | 6529.8805 | 0.0084 |
| 2 | 1 | 1 | 1 | ← | 1 | 0 | 1 | 0 | 6945.1865 | 0.0163 |
| 2 | 1 | 1 | 2 | ← | 1 | 0 | 1 | 2 | 6945.8936 | 0.0050 |
| 2 | 1 | 1 | 3 | ← | 1 | 0 | 1 | 2 | 6946.6602 | 0.0144 |
| 2 | 1 | 1 | 2 | ← | 1 | 0 | 1 | 1 | 6947.1556 | 0.0027 |
| 2 | 1 | 1 | 1 | ← | 1 | 0 | 1 | 1 | 6948.3404 | 0.0088 |
| 7 | 2 | 5 | 8 | ← | 7 | 1 | 6 | 8 | 6994.2407 | 0.0146 |
| 7 | 2 | 5 | 7 | ← | 7 | 1 | 6 | 7 | 6994.4593 | 0.0137 |
| 5 | 2 | 4 | 4 | ← | 5 | 1 | 4 | 4 | 7036.8258 | 0.0085 |
| 5 | 2 | 4 | 5 | ← | 5 | 1 | 4 | 5 | 7037.4485 | 0.0090 |
| 6 | 2 | 4 | 6 | ← | 6 | 1 | 5 | 6 | 7125.4734 | 0.0162 |
| 5 | 2 | 3 | 6 | ← | 5 | 1 | 4 | 6 | 7341.6753 | 0.0127 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 4 | 7388.2353 | -0.0025 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 7389.2024 | -0.0038 |
| 4 | 1 | 4 | 3 | ← | 3 | 1 | 3 | 3 | 7390.6255 | -0.0027 |
| 4 | 2 | 3 | 3 | ← | 4 | 1 | 3 | 3 | 7470.0499 | 0.0092 |
| 4 | 2 | 3 | 5 | ← | 4 | 1 | 3 | 5 | 7470.2273 | 0.0000 |
| 4 | 2 | 3 | 4 | ← | 4 | 1 | 3 | 4 | 7470.9530 | -0.0010 |
| 5 | 0 | 5 | 5 | ← | 4 | 1 | 4 | 5 | 7552.8738 | -0.0098 |
| 5 | 0 | 5 | 5 | ← | 4 | 1 | 4 | 4 | 7554.0008 | -0.0136 |
| 5 | 0 | 5 | 4 | ← | 4 | 1 | 4 | 3 | 7554.2761 | -0.0094 |
| 5 | 0 | 5 | 6 | ← | 4 | 1 | 4 | 5 | 7554.2761 | -0.0139 |
| 5 | 0 | 5 | 4 | ← | 4 | 1 | 4 | 4 | 7555.6948 | -0.0128 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 4 | 7681.4217 | -0.0036 |
| 4 | 0 | 4 | 3 | ← | 3 | 0 | 3 | 2 | 7682.7011 | -0.0021 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 7682.8214 | 0.0101 |
| 4 | 0 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 7682.8214 | -0.0064 |
| 4 | 0 | 4 | 3 | ← | 3 | 0 | 3 | 3 | 7684.5736 | -0.0011 |
| 4 | 2 | 3 | 4 | ← | 3 | 2 | 2 | 3 | 7763.3967 | -0.0006 |
| 4 | 2 | 3 | 4 | ← | 3 | 2 | 2 | 4 | 7763.3967 | -0.0007 |
| 4 | 2 | 3 | 5 | ← | 3 | 2 | 2 | 4 | 7763.9690 | -0.0012 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 2 | 7764.1168 | -0.0005 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 3 | 7764.1168 | -0.0010 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 4 | 7764.1168 | -0.0011 |
| 4 | 3 | 2 | 4 | ← | 3 | 3 | 1 | 3 | 7786.8657 | 0.0135 |
| 4 | 3 | 2 | 5 | ← | 3 | 3 | 1 | 4 | 7788.1268 | 0.0178 |
| 4 | 3 | 1 | 4 | ← | 3 | 3 | 0 | 3 | 7788.5042 | 0.0137 |
| 4 | 3 | 2 | 4 | ← | 3 | 3 | 1 | 4 | 7788.6192 | 0.0130 |
| 4 | 3 | 1 | 5 | ← | 3 | 3 | 0 | 4 | 7789.7590 | 0.0112 |
| 4 | 3 | 1 | 3 | ← | 3 | 3 | 0 | 2 | 7790.2442 | 0.0100 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 2 | 2 | 7822.4017 | -0.0049 |
| 3 | 2 | 2 | 2 | ← | 3 | 1 | 2 | 2 | 7822.4017 | -0.0053 |
| 3 | 2 | 2 | 4 | ← | 3 | 1 | 2 | 4 | 7822.8061 | 0.0022 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 2 | 4 | 7822.8061 | 0.0021 |
| 3 | 2 | 2 | 4 | ← | 3 | 1 | 2 | 3 | 7823.9313 | -0.0065 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 2 | 3 | 7823.9313 | -0.0067 |
| 3 | 2 | 2 | 2 | ← | 3 | 1 | 2 | 3 | 7823.9313 | -0.0071 |
| 4 | 2 | 2 | 4 | ← | 3 | 2 | 1 | 4 | 7851.3484 | 0.0154 |
| 4 | 2 | 2 | 4 | ← | 3 | 2 | 1 | 3 | 7851.3484 | -0.0034 |
| 4 | 2 | 2 | 5 | ← | 3 | 2 | 1 | 4 | 7851.9382 | -0.0019 |
| 4 | 2 | 2 | 3 | ← | 3 | 2 | 1 | 2 | 7852.0851 | -0.0044 |
| 4 | 2 | 2 | 3 | ← | 3 | 2 | 1 | 4 | 7852.0851 | -0.0116 |
| 3 | 2 | 1 | 3 | ← | 3 | 1 | 2 | 2 | 7866.8868 | 0.0187 |
| 3 | 2 | 1 | 3 | ← | 3 | 1 | 2 | 4 | 7867.2764 | 0.0108 |
| 3 | 2 | 1 | 4 | ← | 3 | 1 | 2 | 4 | 7867.2764 | -0.0079 |
| 3 | 2 | 1 | 3 | ← | 3 | 1 | 2 | 3 | 7868.3890 | -0.0105 |
| 3 | 1 | 3 | 3 | ← | 2 | 0 | 2 | 3 | 8071.9170 | 0.0018 |
| 3 | 1 | 3 | 2 | ← | 2 | 0 | 2 | 1 | 8072.4757 | 0.0016 |
| 3 | 1 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 8072.8849 | 0.0012 |
| 3 | 1 | 3 | 3 | ← | 2 | 0 | 2 | 2 | 8073.2656 | 0.0031 |
| 3 | 1 | 3 | 2 | ← | 2 | 0 | 2 | 2 | 8074.5693 | -0.0011 |
| 2 | 2 | 1 | 1 | ← | 2 | 1 | 1 | 1 | 8089.0290 | -0.0056 |
| 2 | 2 | 1 | 3 | ← | 2 | 1 | 1 | 3 | 8090.2118 | 0.0032 |
| 2 | 2 | 1 | 1 | ← | 2 | 1 | 1 | 2 | 8090.2118 | -0.0014 |
| 2 | 2 | 0 | 1 | ← | 2 | 1 | 1 | 1 | 8097.9579 | -0.0059 |
| 2 | 2 | 0 | 3 | ← | 2 | 1 | 1 | 3 | 8099.1292 | -0.0045 |
| 2 | 2 | 0 | 1 | ← | 2 | 1 | 1 | 2 | 8099.1292 | -0.0133 |
| 2 | 2 | 0 | 3 | ← | 2 | 1 | 1 | 2 | 8099.8976 | 0.0066 |
| 2 | 2 | 0 | 2 | ← | 2 | 1 | 1 | 1 | 8100.0554 | -0.0042 |
| 2 | 2 | 0 | 2 | ← | 2 | 1 | 1 | 3 | 8100.4848 | 0.0037 |
| 2 | 2 | 0 | 2 | ← | 2 | 1 | 1 | 2 | 8101.2350 | -0.0033 |
| 4 | 1 | 3 | 4 | ← | 3 | 1 | 2 | 4 | 8115.2411 | -0.0060 |
| 4 | 1 | 3 | 4 | ← | 3 | 1 | 2 | 3 | 8116.3663 | -0.0149 |
| 4 | 1 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 8116.5277 | -0.0190 |
| 4 | 1 | 3 | 3 | ← | 3 | 1 | 2 | 3 | 8118.0139 | -0.0012 |
| 2 | 2 | 1 | 1 | ← | 2 | 1 | 2 | 1 | 8635.7543 | -0.0142 |
| 2 | 2 | 1 | 3 | ← | 2 | 1 | 2 | 3 | 8636.8484 | -0.0056 |
| 2 | 2 | 1 | 3 | ← | 2 | 1 | 2 | 2 | 8637.4301 | -0.0212 |
| 2 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 1 | 8637.8596 | -0.0161 |
| 2 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 3 | 8638.1920 | -0.0167 |
| 2 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 2 | 8638.7937 | -0.0123 |
| 2 | 2 | 0 | 3 | ← | 2 | 1 | 2 | 3 | 8645.7826 | 0.0034 |
| 2 | 2 | 0 | 2 | ← | 2 | 1 | 2 | 2 | 8647.7270 | 0.0032 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 2 | 8915.4607 | 0.0087 |
| 3 | 2 | 2 | 2 | ← | 3 | 1 | 3 | 2 | 8915.4607 | 0.0083 |
| 3 | 2 | 2 | 4 | ← | 3 | 1 | 3 | 4 | 8915.8033 | 0.0118 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 4 | 8915.8033 | 0.0117 |
| 3 | 2 | 2 | 4 | ← | 3 | 1 | 3 | 3 | 8916.7726 | 0.0126 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 3 | 8916.7726 | 0.0125 |
| 3 | 2 | 2 | 2 | ← | 3 | 1 | 3 | 3 | 8916.7726 | 0.0121 |
| 3 | 2 | 1 | 3 | ← | 3 | 1 | 3 | 2 | 8959.9409 | 0.0273 |
| 3 | 2 | 1 | 2 | ← | 3 | 1 | 3 | 2 | 8959.9409 | 0.0012 |
| 3 | 2 | 1 | 4 | ← | 3 | 1 | 3 | 4 | 8960.2899 | 0.0179 |
| 3 | 2 | 1 | 3 | ← | 3 | 1 | 3 | 3 | 8961.2278 | 0.0061 |
| 3 | 2 | 1 | 4 | ← | 3 | 1 | 3 | 3 | 8961.2278 | -0.0126 |
| 3 | 2 | 1 | 2 | ← | 3 | 1 | 3 | 3 | 8961.2278 | -0.0198 |
| 3 | 1 | 2 | 3 | ← | 2 | 0 | 2 | 3 | 9164.7466 | 0.0093 |
| 3 | 1 | 2 | 2 | ← | 2 | 0 | 2 | 1 | 9165.5246 | 0.0052 |
| 3 | 1 | 2 | 4 | ← | 2 | 0 | 2 | 3 | 9165.8780 | 0.0068 |
| 3 | 1 | 2 | 3 | ← | 2 | 0 | 2 | 2 | 9166.0899 | 0.0053 |
| 3 | 1 | 2 | 2 | ← | 2 | 0 | 2 | 2 | 9167.6190 | 0.0031 |
| 5 | 1 | 5 | 5 | ← | 4 | 1 | 4 | 5 | 9220.5013 | 0.0041 |
| 5 | 1 | 5 | 5 | ← | 4 | 1 | 4 | 4 | 9221.6058 | -0.0220 |
| 5 | 1 | 5 | 6 | ← | 4 | 1 | 4 | 5 | 9221.7298 | 0.0157 |
| 5 | 1 | 5 | 4 | ← | 4 | 1 | 4 | 4 | 9223.0884 | -0.0047 |
| 4 | 2 | 3 | 5 | ← | 4 | 1 | 4 | 5 | 9290.4060 | 0.0129 |
| 4 | 2 | 3 | 4 | ← | 4 | 1 | 4 | 4 | 9290.9698 | 0.0187 |

| J' | $K_{a'}$ | $K_{c'}$ | F' | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 5 | 9539.7270 | -0.0044 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 9541.1177 | -0.0163 |
| 5 | 0 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 9541.1177 | -0.0201 |
| 5 | 0 | 5 | 4 | ← | 4 | 0 | 4 | 4 | 9542.8178 | -0.0092 |
| 4 | 1 | 4 | 4 | ← | 3 | 0 | 3 | 4 | 9668.5437 | -0.0010 |
| 4 | 1 | 4 | 3 | ← | 3 | 0 | 3 | 2 | 9669.4819 | 0.0005 |
| 4 | 1 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 9669.6764 | 0.0007 |
| 4 | 1 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 9669.9333 | 0.0025 |
| 4 | 1 | 4 | 3 | ← | 3 | 0 | 3 | 3 | 9671.3363 | -0.0164 |
| 5 | 2 | 4 | 5 | ← | 4 | 2 | 3 | 5 | 9692.8283 | -0.0129 |
| 5 | 2 | 4 | 5 | ← | 4 | 2 | 3 | 4 | 9693.3998 | -0.0141 |
| 5 | 2 | 4 | 4 | ← | 4 | 2 | 3 | 4 | 9694.4509 | -0.0104 |
| 5 | 4 | 1 | 5 | ← | 4 | 4 | 0 | 4 | 9732.4335 | -0.0105 |
| 5 | 4 | 1 | 6 | ← | 4 | 4 | 0 | 5 | 9733.5738 | -0.0094 |
| 5 | 4 | 1 | 4 | ← | 4 | 4 | 0 | 3 | 9733.9098 | -0.0130 |
| 5 | 4 | 2 | 5 | ← | 4 | 4 | 1 | 5 | 9734.3870 | -0.0114 |
| 5 | 3 | 3 | 5 | ← | 4 | 3 | 2 | 4 | 9740.8646 | 0.0124 |
| 5 | 3 | 3 | 6 | ← | 4 | 3 | 2 | 5 | 9741.5156 | 0.0119 |
| 5 | 3 | 2 | 5 | ← | 4 | 3 | 1 | 4 | 9746.5825 | 0.0147 |
| 5 | 3 | 2 | 6 | ← | 4 | 3 | 1 | 5 | 9747.2438 | 0.0230 |
| 5 | 2 | 4 | 6 | ← | 5 | 1 | 5 | 6 | 9762.3902 | -0.0001 |
| 5 | 2 | 4 | 5 | ← | 5 | 1 | 5 | 5 | 9762.7605 | 0.0233 |
| 5 | 2 | 3 | 5 | ← | 4 | 2 | 2 | 5 | 9865.0801 | 0.0025 |
| 5 | 2 | 3 | 5 | ← | 4 | 2 | 2 | 4 | 9865.6840 | -0.0007 |
| 5 | 1 | 4 | 5 | ← | 4 | 1 | 3 | 5 | 10125.6263 | -0.0028 |
| 5 | 1 | 4 | 6 | ← | 4 | 1 | 3 | 5 | 10127.0149 | -0.0010 |
| 5 | 1 | 4 | 4 | ← | 4 | 1 | 3 | 4 | 10128.6031 | 0.0049 |
| 6 | 1 | 6 | 6 | ← | 5 | 1 | 5 | 6 | 11044.1922 | -0.0150 |
| 6 | 1 | 6 | 6 | ← | 5 | 1 | 5 | 5 | 11045.4009 | -0.0232 |
| 6 | 1 | 6 | 5 | ← | 5 | 1 | 5 | 5 | 11046.9101 | 0.0036 |
| 5 | 1 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 11208.5506 | -0.0112 |
| 5 | 1 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 11208.7521 | 0.0047 |
| 6 | 0 | 6 | 6 | ← | 5 | 0 | 5 | 6 | 11363.5658 | -0.0265 |
| 6 | 0 | 6 | 7 | ← | 5 | 0 | 5 | 6 | 11364.9736 | -0.0222 |
| 6 | 0 | 6 | 6 | ← | 5 | 0 | 5 | 5 | 11364.9736 | -0.0252 |
| 6 | 0 | 6 | 5 | ← | 5 | 0 | 5 | 5 | 11366.6141 | -0.0243 |
| 4 | 1 | 3 | 3 | ← | 3 | 0 | 3 | 2 | 11489.7058 | 0.0155 |
| 6 | 2 | 5 | 6 | ← | 5 | 2 | 4 | 6 | 11615.0529 | -0.0004 |
| 6 | 2 | 5 | 6 | ← | 5 | 2 | 4 | 5 | 11615.9348 | 0.0112 |
| 6 | 2 | 5 | 5 | ← | 5 | 2 | 4 | 4 | 11616.0978 | -0.0001 |
| 6 | 2 | 5 | 7 | ← | 5 | 2 | 4 | 6 | 11616.0978 | -0.0005 |
| 6 | 2 | 5 | 5 | ← | 5 | 2 | 4 | 5 | 11617.1574 | 0.0120 |
| 6 | 5 | 2 | 7 | ← | 5 | 5 | 1 | 6 | 11678.6725 | 0.0160 |
| 6 | 5 | 1 | 7 | ← | 5 | 5 | 0 | 6 | 11678.6725 | 0.0144 |
| 6 | 4 | 2 | 7 | ← | 5 | 4 | 1 | 6 | 11686.7590 | -0.0181 |
| 6 | 3 | 4 | 6 | ← | 5 | 3 | 3 | 5 | 11697.6019 | 0.0159 |
| 6 | 3 | 3 | 6 | ← | 5 | 3 | 2 | 5 | 11712.7526 | 0.0152 |
| 6 | 3 | 3 | 7 | ← | 5 | 3 | 2 | 6 | 11713.1484 | 0.0250 |
| 6 | 2 | 4 | 6 | ← | 5 | 2 | 3 | 5 | 11906.8082 | -0.0136 |
| 6 | 2 | 4 | 7 | ← | 5 | 2 | 3 | 6 | 11907.0072 | -0.0088 |
| 6 | 2 | 4 | 5 | ← | 5 | 2 | 3 | 4 | 11907.0072 | -0.0093 |
| 6 | 1 | 5 | 6 | ← | 5 | 1 | 4 | 6 | 12122.0875 | -0.0165 |
| 6 | 1 | 5 | 6 | ← | 5 | 1 | 4 | 5 | 12123.4641 | -0.0268 |
| 6 | 1 | 5 | 5 | ← | 5 | 1 | 4 | 5 | 12125.1593 | -0.0116 |
| 2 | 2 | 1 | 1 | ← | 1 | 1 | 0 | 1 | 12156.7468 | -0.0043 |
| 2 | 2 | 1 | 3 | ← | 1 | 1 | 0 | 2 | 12158.0675 | 0.0066 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 0 | 1 | 12158.8603 | 0.0020 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 0 | 2 | 12159.4141 | -0.0014 |
| 2 | 2 | 1 | 1 | ← | 1 | 1 | 1 | 1 | 12338.8226 | -0.0072 |
| 2 | 2 | 1 | 3 | ← | 1 | 1 | 1 | 2 | 12340.2934 | 0.0044 |
| 2 | 2 | 1 | 1 | ← | 1 | 1 | 1 | 0 | 12340.5965 | 0.0000 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 1 | 1 | 12340.9444 | 0.0073 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 1 | 2 | 12341.6443 | 0.0006 |
| 2 | 2 | 0 | 1 | ← | 1 | 1 | 1 | 1 | 12347.7634 | 0.0043 |
| 2 | 2 | 0 | 3 | ← | 1 | 1 | 1 | 2 | 12349.2223 | 0.0081 |
| 2 | 2 | 0 | 1 | ← | 1 | 1 | 1 | 0 | 12349.5302 | 0.0045 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 1 | 1 | 12349.8621 | 0.0072 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 1 | 2 | 12350.5728 | 0.0113 |
| 6 | 1 | 6 | 6 | ← | 5 | 0 | 5 | 5 | 12713.0368 | -0.0008 |
| 7 | 1 | 7 | 7 | ← | 6 | 1 | 6 | 7 | 12858.8667 | -0.0098 |
| 7 | 1 | 7 | 7 | ← | 6 | 1 | 6 | 6 | 12860.1464 | 0.0019 |
| 7 | 1 | 7 | 6 | ← | 6 | 1 | 6 | 5 | 12860.1464 | -0.0036 |
| 7 | 0 | 7 | 8 | ← | 6 | 0 | 6 | 7 | 13156.8139 | -0.0010 |
| 7 | 0 | 7 | 7 | ← | 6 | 0 | 6 | 6 | 13156.8139 | -0.0085 |
| 7 | 2 | 6 | 8 | ← | 6 | 2 | 5 | 7 | 13529.7421 | 0.0126 |
| 7 | 2 | 6 | 6 | ← | 6 | 2 | 5 | 5 | 13529.7421 | 0.0224 |
| 7 | 4 | 3 | 8 | ← | 6 | 4 | 2 | 7 | 13643.7885 | -0.0215 |
| 7 | 3 | 5 | 7 | ← | 6 | 3 | 4 | 6 | 13656.5649 | -0.0090 |
| 7 | 3 | 5 | 8 | ← | 6 | 3 | 4 | 7 | 13656.8237 | 0.0042 |
| 7 | 3 | 4 | 7 | ← | 6 | 3 | 3 | 6 | 13690.3420 | 0.0161 |
| 7 | 3 | 4 | 6 | ← | 6 | 3 | 3 | 5 | 13690.6079 | 0.0096 |
| 4 | 3 | 1 | 4 | ← | 4 | 2 | 2 | 4 | 13839.6644 | -0.0098 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 1 | 13918.1568 | -0.0058 |
| 3 | 2 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 13918.5860 | 0.0025 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 1 | 3 | 13918.5860 | 0.0023 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 3 | 13918.5860 | 0.0019 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 13919.3451 | 0.0043 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 2 | 13919.3451 | 0.0038 |
| 5 | 1 | 4 | 5 | ← | 4 | 0 | 4 | 4 | 13934.0578 | 0.0127 |
| 3 | 2 | 1 | 2 | ← | 2 | 1 | 1 | 1 | 13962.6376 | -0.0121 |
| 3 | 2 | 1 | 3 | ← | 2 | 1 | 1 | 3 | 13963.0570 | 0.0118 |
| 3 | 2 | 1 | 3 | ← | 2 | 1 | 1 | 2 | 13963.7931 | -0.0092 |
| 4 | 3 | 2 | 5 | ← | 4 | 2 | 3 | 4 | 13969.6857 | 0.0044 |
| 7 | 2 | 5 | 6 | ← | 6 | 2 | 4 | 5 | 13970.9023 | -0.0136 |
| 7 | 2 | 5 | 8 | ← | 6 | 2 | 4 | 7 | 13970.9023 | -0.0224 |
| 7 | 1 | 6 | 6 | ← | 6 | 1 | 5 | 5 | 14101.7888 | -0.0161 |
| 7 | 1 | 6 | 7 | ← | 6 | 1 | 5 | 6 | 14101.7888 | -0.0178 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 2 | 1 | 14464.9044 | 0.0079 |
| 3 | 2 | 2 | 4 | ← | 2 | 1 | 2 | 3 | 14465.2461 | 0.0172 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 2 | 3 | 14465.2461 | 0.0170 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 2 | 3 | 14465.2461 | 0.0166 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 2 | 2 | 14465.8432 | 0.0168 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 2 | 2 | 14465.8432 | 0.0164 |
| 3 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 1 | 14509.3715 | -0.0121 |
| 3 | 2 | 1 | 3 | ← | 2 | 1 | 2 | 3 | 14509.6995 | 0.0089 |
| 3 | 2 | 1 | 3 | ← | 2 | 1 | 2 | 2 | 14510.2767 | -0.0111 |
| 8 | 1 | 8 | 7 | ← | 7 | 1 | 7 | 6 | 14665.8203 | -0.0108 |
| 8 | 1 | 8 | 8 | ← | 7 | 1 | 7 | 7 | 14665.8203 | -0.0109 |
| 8 | 0 | 8 | 8 | ← | 7 | 0 | 7 | 8 | 14922.1357 | -0.0022 |
| 8 | 0 | 8 | 7 | ← | 7 | 0 | 7 | 6 | 14923.5031 | 0.0035 |
| 8 | 0 | 8 | 9 | ← | 7 | 0 | 7 | 8 | 14923.5031 | -0.0230 |
| 8 | 2 | 7 | 7 | ← | 7 | 2 | 6 | 6 | 15433.2723 | -0.0211 |
| 4 | 2 | 3 | 3 | ← | 3 | 1 | 2 | 2 | 15586.5168 | -0.0076 |
| 4 | 2 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 15586.7560 | -0.0181 |
| 4 | 2 | 3 | 4 | ← | 3 | 1 | 2 | 3 | 15587.3246 | -0.0107 |
| 8 | 4 | 4 | 9 | ← | 7 | 4 | 3 | 8 | 15605.5188 | -0.0073 |
| 8 | 1 | 8 | 9 | ← | 7 | 0 | 7 | 8 | 15717.1119 | -0.0054 |
| 4 | 2 | 2 | 3 | ← | 3 | 1 | 2 | 2 | 15718.9706 | -0.0130 |
| 4 | 2 | 2 | 5 | ← | 3 | 1 | 2 | 4 | 15719.2009 | -0.0235 |
| 8 | 2 | 6 | 8 | ← | 7 | 2 | 5 | 7 | 16048.9497 | 0.0187 |
| 8 | 1 | 7 | 7 | ← | 7 | 1 | 6 | 6 | 16056.9834 | 0.0223 |
| 8 | 1 | 7 | 8 | ← | 7 | 1 | 6 | 7 | 16056.9834 | 0.0136 |
| 8 | 1 | 7 | 9 | ← | 7 | 1 | 6 | 8 | 16056.9834 | -0.0024 |
| 9 | 1 | 9 | 10 | ← | 8 | 1 | 8 | 9 | 16462.9970 | 0.0141 |
| 4 | 2 | 3 | 5 | ← | 3 | 1 | 3 | 4 | 16679.7711 | 0.0093 |
| 4 | 2 | 3 | 4 | ← | 3 | 1 | 3 | 3 | 16680.1841 | 0.0267 |
| 4 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 2 | 16812.0260 | -0.0030 |
| 4 | 2 | 2 | 5 | ← | 3 | 1 | 3 | 4 | 16812.2194 | 0.0073 |
| 4 | 2 | 2 | 4 | ← | 3 | 1 | 3 | 3 | 16812.5621 | -0.0113 |
| 5 | 2 | 4 | 6 | ← | 4 | 1 | 3 | 5 | 17163.9303 | -0.0085 |
| 5 | 2 | 4 | 5 | ← | 4 | 1 | 3 | 4 | 17164.3651 | -0.0029 |
| 9 | 2 | 8 | 9 | ← | 8 | 2 | 7 | 8 | 17325.6291 | -0.0021 |
| 5 | 2 | 3 | 5 | ← | 4 | 1 | 3 | 4 | 17469.0419 | -0.0129 |
| 9 | 4 | 5 | 10 | ← | 8 | 4 | 4 | 9 | 17572.9883 | -0.0091 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | 1 | 8 | 8 | ← | 8 | 1 | 7 | 7 | 17983.7033 | 0.0281 |
| 9 | 1 | 8 | 9 | ← | 8 | 1 | 7 | 8 | 17983.7033 | 0.0146 |
| 9 | 1 | 8 | 10 | ← | 8 | 1 | 7 | 9 | 17983.7033 | 0.0078 |
| 9 | 2 | 7 | 8 | ← | 8 | 2 | 6 | 7 | 18130.1781 | 0.0048 |
| 9 | 2 | 7 | 10 | ← | 8 | 2 | 6 | 9 | 18130.1781 | -0.0068 |
| 9 | 2 | 7 | 8 | ← | 8 | 2 | 6 | 8 | 18131.6703 | -0.0096 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 10 | 18251.0540 | 0.0092 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 18252.3882 | 0.0122 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 18252.3882 | 0.0079 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 18252.3882 | -0.0019 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 18417.4987 | 0.0178 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 18417.4987 | 0.0016 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 18417.4987 | -0.0035 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 9 | 18419.0385 | 0.0217 |
| 6 | 2 | 5 | 6 | ← | 5 | 1 | 4 | 5 | 18653.3912 | 0.0282 |
| 10 | 1 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 18834.7100 | 0.0305 |
| 10 | 1 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 18834.7100 | 0.0113 |
| 5 | 2 | 4 | 6 | ← | 4 | 1 | 4 | 5 | 18984.1223 | 0.0178 |
| 10 | 4 | 6 | 10 | ← | 10 | 3 | 7 | 10 | 19027.7438 | -0.0035 |
| 4 | 2 | 2 | 4 | ← | 3 | 0 | 3 | 3 | 19093.3251 | 0.0272 |
| 10 | 2 | 9 | 10 | ← | 9 | 2 | 8 | 9 | 19205.9146 | 0.0243 |
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 8 | 19205.9146 | -0.0006 |
| 10 | 2 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 19205.9146 | -0.0114 |
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 9 | 19207.3288 | -0.0099 |
| 9 | 4 | 5 | 8 | ← | 9 | 3 | 6 | 8 | 19210.8746 | -0.0095 |
| 9 | 4 | 5 | 9 | ← | 9 | 3 | 6 | 9 | 19211.2714 | -0.0287 |
| 7 | 1 | 6 | 8 | ← | 6 | 0 | 6 | 7 | 19253.2846 | 0.0115 |
| 5 | 2 | 3 | 4 | ← | 4 | 1 | 4 | 5 | 19289.0133 | -0.0193 |
| 8 | 4 | 4 | 7 | ← | 8 | 3 | 5 | 7 | 19333.4338 | -0.0041 |
| 10 | 4 | 7 | 9 | ← | 10 | 3 | 8 | 9 | 19446.1279 | -0.0151 |
| 10 | 4 | 7 | 10 | ← | 10 | 3 | 8 | 10 | 19446.4328 | -0.0258 |
| 8 | 4 | 5 | 7 | ← | 8 | 3 | 6 | 7 | 19452.9945 | -0.0303 |
| 8 | 4 | 4 | 7 | ← | 8 | 3 | 6 | 7 | 19456.4243 | -0.0141 |
| 6 | 4 | 2 | 7 | ← | 6 | 3 | 3 | 7 | 19458.0474 | -0.0307 |
| 5 | 4 | 2 | 5 | ← | 5 | 3 | 2 | 5 | 19485.3750 | -0.0141 |
| 5 | 4 | 1 | 4 | ← | 5 | 3 | 3 | 4 | 19491.8208 | -0.0241 |
| 4 | 4 | 0 | 5 | ← | 4 | 3 | 2 | 4 | 19499.4624 | -0.0147 |
| 10 | 4 | 7 | 11 | ← | 9 | 4 | 6 | 10 | 19536.0216 | 0.0314 |
| 10 | 4 | 7 | 9 | ← | 9 | 4 | 6 | 8 | 19536.0216 | 0.0242 |
| 10 | 4 | 6 | 11 | ← | 9 | 4 | 5 | 10 | 19547.6343 | 0.0228 |
| 10 | 4 | 6 | 9 | ← | 9 | 4 | 5 | 8 | 19547.6343 | 0.0155 |
| 10 | 3 | 7 | 9 | ← | 9 | 3 | 6 | 8 | 19731.1336 | 0.0271 |
| 10 | 3 | 7 | 11 | ← | 9 | 3 | 6 | 10 | 19731.1336 | 0.0246 |
| 11 | 0 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 19742.0022 | 0.0079 |
| 11 | 0 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 19742.0022 | -0.0093 |
| 11 | 0 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 19742.0022 | -0.0192 |
| 3 | 3 | 1 | 4 | ← | 2 | 2 | 0 | 3 | 19764.3997 | -0.0199 |
| 3 | 3 | 0 | 3 | ← | 2 | 2 | 1 | 2 | 19774.0126 | -0.0047 |
| 3 | 3 | 0 | 3 | ← | 2 | 2 | 1 | 3 | 19775.3530 | -0.0190 |
| 10 | 1 | 9 | 10 | ← | 9 | 1 | 8 | 10 | 19875.4204 | -0.0078 |
| 10 | 1 | 9 | 9 | ← | 9 | 1 | 8 | 8 | 19876.8963 | -0.0041 |
| 10 | 1 | 9 | 11 | ← | 9 | 1 | 8 | 10 | 19876.8963 | -0.0209 |
| 10 | 1 | 9 | 10 | ← | 9 | 1 | 8 | 9 | 19876.8963 | -0.0212 |
| 10 | 1 | 9 | 9 | ← | 9 | 1 | 8 | 9 | 19878.5470 | -0.0095 |
| 11 | 1 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 20035.1086 | 0.0115 |
| 11 | 1 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 20035.1086 | 0.0067 |
| 11 | 1 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 20035.1086 | -0.0001 |
| 11 | 0 | 11 | 10 | ← | 10 | 0 | 10 | 9 | 20159.2254 | 0.0153 |
| 11 | 0 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 20159.2254 | 0.0023 |
| 11 | 0 | 11 | 11 | ← | 10 | 0 | 10 | 10 | 20159.2254 | -0.0011 |
| 10 | 2 | 8 | 10 | ← | 9 | 2 | 7 | 9 | 20203.6099 | 0.0044 |
| 10 | 2 | 8 | 9 | ← | 9 | 2 | 7 | 8 | 20203.6099 | -0.0309 |
| 11 | 1 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 20452.3342 | 0.0238 |
| 11 | 1 | 11 | 11 | ← | 10 | 0 | 10 | 10 | 20452.3342 | 0.0000 |
| 11 | 2 | 10 | 11 | ← | 10 | 2 | 9 | 10 | 21073.3644 | 0.0142 |
| 11 | 2 | 10 | 10 | ← | 10 | 2 | 9 | 9 | 21073.3644 | -0.0015 |
| 11 | 2 | 10 | 12 | ← | 10 | 2 | 9 | 11 | 21073.3644 | -0.0113 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | 2 | 5 | 6 | ← | 5 | 1 | 5 | 5 | 21378.6504 | -0.0102 |
| 6 | 2 | 5 | 5 | ← | 5 | 1 | 5 | 6 | 21378.6504 | -0.0151 |
| 11 | 5 | 6 | 10 | ← | 10 | 5 | 5 | 9 | 21469.0718 | 0.0305 |
| 11 | 3 | 9 | 10 | ← | 10 | 3 | 8 | 9 | 21486.8434 | 0.0153 |
| 11 | 3 | 9 | 12 | ← | 10 | 3 | 8 | 11 | 21486.8434 | 0.0106 |
| 11 | 4 | 7 | 10 | ← | 10 | 4 | 6 | 9 | 21531.2084 | 0.0324 |
| 12 | 0 | 12 | 12 | ← | 11 | 1 | 11 | 11 | 21609.6379 | 0.0023 |
| 12 | 0 | 12 | 11 | ← | 11 | 1 | 11 | 10 | 21609.6379 | -0.0069 |
| 12 | 0 | 12 | 13 | ← | 11 | 1 | 11 | 12 | 21609.6379 | -0.0158 |
| 4 | 3 | 2 | 4 | ← | 3 | 2 | 1 | 4 | 21689.0847 | -0.0108 |
| 4 | 3 | 2 | 4 | ← | 3 | 2 | 1 | 3 | 21689.0847 | -0.0296 |
| 4 | 3 | 1 | 4 | ← | 3 | 2 | 1 | 4 | 21691.0315 | 0.0244 |
| 4 | 3 | 1 | 4 | ← | 3 | 2 | 1 | 3 | 21691.0315 | 0.0055 |
| 11 | 1 | 10 | 10 | ← | 10 | 1 | 9 | 9 | 21732.9210 | -0.0110 |
| 11 | 1 | 10 | 12 | ← | 10 | 1 | 9 | 11 | 21732.9210 | -0.0253 |
| 11 | 1 | 10 | 11 | ← | 10 | 1 | 9 | 10 | 21732.9210 | -0.0308 |
| 4 | 3 | 2 | 3 | ← | 3 | 2 | 2 | 2 | 21732.9210 | -0.0297 |
| 4 | 3 | 2 | 3 | ← | 3 | 2 | 2 | 3 | 21732.9210 | -0.0301 |
| 4 | 3 | 2 | 3 | ← | 3 | 2 | 2 | 4 | 21732.9210 | -0.0303 |
| 4 | 3 | 2 | 4 | ← | 3 | 2 | 2 | 3 | 21733.5425 | -0.0334 |
| 4 | 3 | 2 | 4 | ← | 3 | 2 | 2 | 4 | 21733.5425 | -0.0335 |
| 4 | 3 | 1 | 5 | ← | 3 | 2 | 2 | 4 | 21734.9883 | -0.0029 |
| 4 | 3 | 1 | 4 | ← | 3 | 2 | 2 | 3 | 21735.4881 | 0.0005 |
| 4 | 3 | 1 | 4 | ← | 3 | 2 | 2 | 4 | 21735.4881 | 0.0004 |
| 11 | 3 | 8 | 10 | ← | 10 | 3 | 7 | 9 | 21792.4453 | 0.0044 |
| 11 | 3 | 8 | 12 | ← | 10 | 3 | 7 | 11 | 21792.4453 | 0.0006 |
| 12 | 1 | 12 | 11 | ← | 11 | 1 | 11 | 10 | 21812.2630 | 0.0144 |
| 12 | 1 | 12 | 12 | ← | 11 | 1 | 11 | 11 | 21812.2630 | 0.0094 |
| 12 | 1 | 12 | 13 | ← | 11 | 1 | 11 | 12 | 21812.2630 | 0.0044 |
| 12 | 0 | 12 | 11 | ← | 11 | 0 | 11 | 10 | 21902.7479 | 0.0175 |
| 12 | 0 | 12 | 13 | ← | 11 | 0 | 11 | 12 | 21902.7479 | 0.0068 |
| 12 | 0 | 12 | 12 | ← | 11 | 0 | 11 | 11 | 21902.7479 | 0.0047 |
| 6 | 2 | 4 | 6 | ← | 5 | 1 | 5 | 6 | 21973.0215 | -0.0072 |
| 6 | 2 | 4 | 7 | ← | 5 | 1 | 5 | 6 | 21974.1330 | -0.0131 |
| 6 | 2 | 4 | 5 | ← | 5 | 1 | 5 | 6 | 21974.3528 | 0.0177 |
| 12 | 1 | 12 | 13 | ← | 11 | 0 | 11 | 12 | 22105.3697 | 0.0238 |
| 12 | 1 | 12 | 12 | ← | 11 | 0 | 11 | 11 | 22105.3697 | 0.0086 |
| 8 | 1 | 7 | 9 | ← | 7 | 0 | 7 | 8 | 22153.4683 | 0.0241 |
| 11 | 2 | 9 | 11 | ← | 10 | 2 | 8 | 10 | 22260.6459 | -0.0244 |
| 12 | 2 | 11 | 12 | ← | 11 | 2 | 10 | 11 | 22927.6781 | -0.0009 |
| 12 | 2 | 11 | 11 | ← | 11 | 2 | 10 | 10 | 22927.6781 | -0.0105 |
| 12 | 2 | 11 | 13 | ← | 11 | 2 | 10 | 12 | 22927.6781 | -0.0192 |
| 12 | 3 | 10 | 12 | ← | 11 | 3 | 9 | 11 | 23433.1135 | 0.0312 |
| 12 | 3 | 10 | 11 | ← | 11 | 3 | 9 | 10 | 23433.1135 | -0.0136 |
| 12 | 3 | 10 | 13 | ← | 11 | 3 | 9 | 12 | 23433.1135 | -0.0187 |
| 13 | 0 | 13 | 13 | ← | 12 | 1 | 12 | 12 | 23446.7136 | 0.0025 |
| 13 | 0 | 13 | 12 | ← | 12 | 1 | 12 | 11 | 23446.7136 | -0.0017 |
| 13 | 0 | 13 | 14 | ← | 12 | 1 | 12 | 13 | 23446.7136 | -0.0096 |
| 12 | 1 | 11 | 11 | ← | 11 | 1 | 10 | 10 | 23550.7898 | -0.0138 |
| 12 | 1 | 11 | 13 | ← | 11 | 1 | 10 | 12 | 23550.7898 | -0.0260 |
| 12 | 1 | 11 | 11 | ← | 11 | 1 | 10 | 11 | 23552.4280 | 0.0052 |
| 5 | 3 | 3 | 6 | ← | 4 | 2 | 2 | 5 | 23578.1766 | 0.0148 |
| 5 | 3 | 3 | 5 | ← | 4 | 2 | 2 | 4 | 23578.6062 | -0.0084 |
| 13 | 1 | 13 | 12 | ← | 12 | 1 | 12 | 11 | 23584.9397 | 0.0138 |
| 13 | 1 | 13 | 13 | ← | 12 | 1 | 12 | 12 | 23584.9397 | 0.0090 |
| 13 | 1 | 13 | 14 | ← | 12 | 1 | 12 | 13 | 23584.9397 | 0.0053 |
| 5 | 3 | 2 | 4 | ← | 4 | 2 | 2 | 5 | 23585.8190 | -0.0045 |
| 5 | 3 | 2 | 5 | ← | 4 | 2 | 2 | 4 | 23586.2354 | -0.0065 |
| 13 | 0 | 13 | 12 | ← | 12 | 0 | 12 | 11 | 23649.3336 | 0.0146 |
| 13 | 0 | 13 | 14 | ← | 12 | 0 | 12 | 13 | 23649.3336 | 0.0056 |
| 13 | 0 | 13 | 13 | ← | 12 | 0 | 12 | 12 | 23649.3336 | 0.0046 |
| 5 | 3 | 3 | 6 | ← | 4 | 2 | 3 | 5 | 23710.5937 | -0.0185 |
| 5 | 3 | 3 | 5 | ← | 4 | 2 | 3 | 4 | 23711.0167 | -0.0139 |
| 5 | 3 | 2 | 6 | ← | 4 | 2 | 3 | 5 | 23718.2285 | -0.0131 |
| 5 | 3 | 2 | 5 | ← | 4 | 2 | 3 | 4 | 23718.6579 | 0.0000 |
| 13 | 1 | 13 | 12 | ← | 12 | 0 | 12 | 11 | 23787.5608 | 0.0313 |
| 13 | 1 | 13 | 14 | ← | 12 | 0 | 12 | 13 | 23787.5608 | 0.0217 |

| J' | $K_{a'}$ | $K_{c'}$ | F' | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | 1 | 13 | 13 | ← | 12 | 0 | 12 | 12 | 23787.5608 | 0.0122 |
| 12 | 3 | 9 | 12 | ← | 11 | 3 | 8 | 11 | 23879.1862 | 0.0233 |
| 13 | 2 | 12 | 13 | ← | 12 | 2 | 11 | 12 | 24768.9006 | -0.0098 |
| 13 | 2 | 12 | 12 | ← | 12 | 2 | 11 | 11 | 24768.9006 | -0.0150 |
| 13 | 2 | 12 | 14 | ← | 12 | 2 | 11 | 13 | 24768.9006 | -0.0228 |
| 9 | 2 | 7 | 10 | ← | 8 | 1 | 7 | 9 | 25116.4528 | 0.0058 |
| 9 | 1 | 8 | 10 | ← | 8 | 0 | 8 | 9 | 25213.6281 | 0.0148 |
| 14 | 0 | 14 | 14 | ← | 13 | 1 | 13 | 13 | 25260.8867 | 0.0139 |
| 14 | 0 | 14 | 13 | ← | 13 | 1 | 13 | 12 | 25260.8867 | 0.0127 |
| 14 | 0 | 14 | 15 | ← | 13 | 1 | 13 | 14 | 25260.8867 | 0.0057 |
| 13 | 1 | 12 | 12 | ← | 12 | 1 | 11 | 11 | 25333.3791 | -0.0335 |
| 14 | 1 | 14 | 13 | ← | 13 | 1 | 13 | 12 | 25354.1114 | -0.0121 |
| 14 | 1 | 14 | 14 | ← | 13 | 1 | 13 | 13 | 25354.1114 | -0.0167 |
| 14 | 1 | 14 | 15 | ← | 13 | 1 | 13 | 14 | 25354.1114 | -0.0195 |
| 13 | 3 | 11 | 13 | ← | 12 | 3 | 10 | 12 | 25370.6799 | -0.0146 |
| 14 | 0 | 14 | 13 | ← | 13 | 0 | 13 | 12 | 25399.0926 | 0.0081 |
| 14 | 0 | 14 | 15 | ← | 13 | 0 | 13 | 14 | 25399.0926 | 0.0004 |
| 14 | 0 | 14 | 14 | ← | 13 | 0 | 13 | 13 | 25399.0926 | 0.0002 |
| 6 | 3 | 4 | 6 | ← | 5 | 2 | 3 | 5 | 25410.5275 | 0.0116 |
| 6 | 3 | 3 | 6 | ← | 5 | 2 | 3 | 5 | 25433.3014 | 0.0068 |
| 13 | 4 | 10 | 12 | ← | 12 | 4 | 9 | 11 | 25461.5494 | 0.0096 |
| 13 | 4 | 10 | 14 | ← | 12 | 4 | 9 | 13 | 25461.5494 | 0.0081 |
| 13 | 4 | 9 | 12 | ← | 12 | 4 | 8 | 11 | 25534.9535 | -0.0215 |
| 13 | 4 | 9 | 14 | ← | 12 | 4 | 8 | 13 | 25534.9535 | -0.0227 |
| 6 | 3 | 4 | 6 | ← | 5 | 2 | 4 | 5 | 25715.2042 | 0.0015 |
| 6 | 3 | 3 | 6 | ← | 5 | 2 | 4 | 5 | 25737.9954 | 0.0140 |
| 13 | 3 | 10 | 13 | ← | 12 | 3 | 9 | 12 | 25987.0385 | -0.0311 |
| | | | | | | | | | RMS | 12.5 kHz |

Table S10 Linelist for Conformer II of isoleucinol. OMC is the difference between the observed and calculated transition.

| J' | $K_{a'}$ | $K_{c'}$ | F' | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 1 | 1 | ← | 0 | 0 | 0 | 1 | 2074.1552 | -0.0006 |
| 1 | 0 | 1 | 2 | ← | 0 | 0 | 0 | 1 | 2075.4239 | 0.0035 |
| 1 | 0 | 1 | 0 | ← | 0 | 0 | 0 | 1 | 2077.3184 | 0.0008 |
| 1 | 1 | 0 | 2 | ← | 1 | 0 | 1 | 2 | 2198.3141 | 0.0122 |
| 1 | 1 | 0 | 0 | ← | 1 | 0 | 1 | 1 | 2198.5123 | 0.0100 |
| 1 | 1 | 0 | 2 | ← | 1 | 0 | 1 | 1 | 2199.5809 | 0.0145 |
| 2 | 1 | 1 | 3 | ← | 2 | 0 | 2 | 3 | 2336.6198 | 0.0080 |
| 2 | 1 | 1 | 3 | ← | 2 | 0 | 2 | 2 | 2337.9859 | 0.0161 |
| 3 | 1 | 2 | 3 | ← | 3 | 0 | 3 | 4 | 2554.2224 | -0.0086 |
| 3 | 1 | 2 | 2 | ← | 3 | 0 | 3 | 2 | 2555.0590 | 0.0142 |
| 3 | 1 | 2 | 4 | ← | 3 | 0 | 3 | 4 | 2555.2138 | 0.0137 |
| 3 | 1 | 2 | 3 | ← | 3 | 0 | 3 | 3 | 2555.6588 | 0.0145 |
| 4 | 1 | 3 | 3 | ← | 4 | 0 | 4 | 3 | 2866.8779 | 0.0105 |
| 4 | 1 | 3 | 5 | ← | 4 | 0 | 4 | 5 | 2866.9590 | 0.0105 |
| 4 | 1 | 3 | 4 | ← | 4 | 0 | 4 | 4 | 2867.2763 | 0.0123 |
| 5 | 1 | 4 | 6 | ← | 5 | 0 | 5 | 6 | 3287.0070 | -0.0068 |
| 2 | 1 | 2 | 2 | ← | 1 | 1 | 1 | 1 | 4017.3442 | 0.0028 |
| 2 | 1 | 2 | 2 | ← | 1 | 1 | 1 | 2 | 4017.8936 | -0.0026 |
| 2 | 1 | 2 | 1 | ← | 1 | 1 | 1 | 1 | 4018.5252 | 0.0005 |
| 2 | 1 | 2 | 3 | ← | 1 | 1 | 1 | 2 | 4018.6553 | -0.0009 |
| 2 | 1 | 2 | 1 | ← | 1 | 1 | 1 | 0 | 4019.9096 | -0.0022 |
| 1 | 1 | 1 | 0 | ← | 0 | 0 | 0 | 1 | 4140.9050 | 0.0133 |
| 1 | 1 | 1 | 2 | ← | 0 | 0 | 0 | 1 | 4141.7400 | 0.0158 |
| 1 | 1 | 1 | 1 | ← | 0 | 0 | 0 | 1 | 4142.2855 | 0.0065 |
| 2 | 0 | 2 | 2 | ← | 1 | 0 | 1 | 2 | 4143.0239 | -0.0005 |
| 2 | 0 | 2 | 1 | ← | 1 | 0 | 1 | 0 | 4143.2428 | 0.0025 |
| 2 | 0 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 4144.3804 | -0.0019 |
| 2 | 0 | 2 | 1 | ← | 1 | 0 | 1 | 1 | 4146.4006 | -0.0013 |
| 3 | 0 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 4260.0107 | -0.0156 |
| 3 | 0 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 4260.6607 | -0.0189 |
| 3 | 0 | 3 | 2 | ← | 2 | 1 | 2 | 1 | 4260.7515 | 0.0000 |
| 1 | 1 | 0 | 0 | ← | 0 | 0 | 0 | 1 | 4272.6687 | 0.0105 |
| 1 | 1 | 0 | 2 | ← | 0 | 0 | 0 | 1 | 4273.7300 | 0.0078 |
| 1 | 1 | 0 | 1 | ← | 0 | 0 | 0 | 1 | 4274.4449 | 0.0134 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 1 | 1 | 2 | ← | 1 | 1 | 0 | 1 | 4281.3850 | -0.0034 |
| 2 | 1 | 1 | 2 | ← | 1 | 1 | 0 | 2 | 4282.0966 | -0.0010 |
| 2 | 1 | 1 | 1 | ← | 1 | 1 | 0 | 1 | 4282.3128 | -0.0014 |
| 2 | 1 | 1 | 3 | ← | 1 | 1 | 0 | 2 | 4282.6898 | -0.0024 |
| 2 | 1 | 1 | 1 | ← | 1 | 1 | 0 | 0 | 4284.0891 | 0.0015 |
| 5 | 2 | 4 | 4 | ← | 5 | 1 | 4 | 4 | 5434.6148 | 0.0056 |
| 5 | 2 | 4 | 5 | ← | 5 | 1 | 4 | 5 | 5435.0498 | 0.0173 |
| 6 | 2 | 4 | 6 | ← | 6 | 1 | 5 | 6 | 5476.2151 | -0.0136 |
| 5 | 2 | 3 | 4 | ← | 5 | 1 | 4 | 4 | 5644.2702 | -0.0106 |
| 5 | 2 | 3 | 6 | ← | 5 | 1 | 4 | 6 | 5644.3503 | -0.0068 |
| 5 | 2 | 3 | 5 | ← | 5 | 1 | 4 | 5 | 5644.7221 | -0.0100 |
| 4 | 0 | 4 | 4 | ← | 3 | 1 | 2 | 3 | 5684.6887 | -0.0054 |
| 4 | 0 | 4 | 5 | ← | 3 | 1 | 2 | 4 | 5685.1841 | 0.0069 |
| 4 | 2 | 3 | 3 | ← | 4 | 1 | 3 | 3 | 5749.4172 | -0.0060 |
| 4 | 2 | 3 | 5 | ← | 4 | 1 | 3 | 5 | 5749.5720 | 0.0045 |
| 4 | 2 | 3 | 4 | ← | 4 | 1 | 3 | 4 | 5750.1241 | -0.0043 |
| 4 | 2 | 2 | 3 | ← | 4 | 1 | 3 | 3 | 5840.4129 | -0.0119 |
| 4 | 2 | 2 | 5 | ← | 4 | 1 | 3 | 5 | 5840.5655 | -0.0074 |
| 4 | 2 | 2 | 4 | ← | 4 | 1 | 3 | 4 | 5841.1390 | -0.0097 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 2 | 2 | 6005.1239 | -0.0138 |
| 3 | 2 | 2 | 2 | ← | 3 | 1 | 2 | 2 | 6005.1239 | -0.0142 |
| 3 | 2 | 2 | 4 | ← | 3 | 1 | 2 | 4 | 6005.4859 | 0.0085 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 2 | 4 | 6005.4859 | 0.0084 |
| 3 | 2 | 2 | 4 | ← | 3 | 1 | 2 | 3 | 6006.4407 | -0.0055 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 2 | 3 | 6006.4407 | -0.0056 |
| 3 | 2 | 2 | 2 | ← | 3 | 1 | 2 | 3 | 6006.4407 | -0.0060 |
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 3 | 6022.8210 | 0.0009 |
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 6023.5817 | 0.0015 |
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 6023.9698 | 0.0091 |
| 3 | 1 | 3 | 2 | ← | 2 | 1 | 2 | 2 | 6025.1269 | 0.0065 |
| 3 | 2 | 1 | 4 | ← | 3 | 1 | 2 | 4 | 6036.0107 | -0.0043 |
| 3 | 2 | 1 | 3 | ← | 3 | 1 | 2 | 4 | 6036.0107 | -0.0126 |
| 3 | 2 | 1 | 2 | ← | 3 | 1 | 2 | 3 | 6036.9881 | 0.0063 |
| 3 | 2 | 1 | 4 | ← | 3 | 1 | 2 | 3 | 6036.9881 | 0.0040 |
| 3 | 2 | 1 | 3 | ← | 3 | 1 | 2 | 3 | 6036.9881 | -0.0042 |
| 2 | 1 | 2 | 1 | ← | 1 | 0 | 1 | 0 | 6083.5006 | 0.0145 |
| 2 | 1 | 2 | 2 | ← | 1 | 0 | 1 | 2 | 6084.2137 | 0.0136 |
| 2 | 1 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 6084.9737 | 0.0136 |
| 2 | 1 | 2 | 2 | ← | 1 | 0 | 1 | 1 | 6085.4728 | 0.0083 |
| 2 | 1 | 2 | 1 | ← | 1 | 0 | 1 | 1 | 6086.6591 | 0.0113 |
| 3 | 0 | 3 | 3 | ← | 2 | 0 | 2 | 3 | 6199.8473 | 0.0032 |
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 1 | 6201.0006 | 0.0033 |
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 6201.2535 | -0.0038 |
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 2 | 6203.1150 | 0.0046 |
| 2 | 2 | 0 | 1 | ← | 2 | 1 | 1 | 1 | 6204.4280 | -0.0041 |
| 2 | 2 | 0 | 2 | ← | 2 | 1 | 1 | 2 | 6207.4615 | -0.0088 |
| 3 | 2 | 2 | 3 | ← | 2 | 2 | 1 | 2 | 6224.5846 | 0.0094 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 2 | 6224.5846 | 0.0090 |
| 3 | 2 | 2 | 4 | ← | 2 | 2 | 1 | 3 | 6225.9456 | 0.0156 |
| 3 | 2 | 2 | 3 | ← | 2 | 2 | 1 | 3 | 6225.9456 | 0.0155 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 3 | 6225.9456 | 0.0151 |
| 3 | 2 | 1 | 2 | ← | 2 | 2 | 0 | 2 | 6248.9769 | -0.0057 |
| 3 | 2 | 1 | 3 | ← | 2 | 2 | 0 | 2 | 6248.9769 | -0.0163 |
| 3 | 2 | 1 | 2 | ← | 2 | 2 | 0 | 3 | 6250.3304 | -0.0102 |
| 3 | 2 | 1 | 4 | ← | 2 | 2 | 0 | 3 | 6250.3304 | -0.0126 |
| 3 | 2 | 1 | 2 | ← | 2 | 2 | 0 | 1 | 6251.0855 | -0.0094 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 3 | 6418.8762 | -0.0004 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 6419.4699 | -0.0012 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6419.8443 | -0.0012 |
| 3 | 1 | 2 | 2 | ← | 2 | 1 | 1 | 1 | 6419.8443 | -0.0097 |
| 3 | 1 | 2 | 2 | ← | 2 | 1 | 1 | 2 | 6420.7754 | -0.0045 |
| 4 | 0 | 4 | 4 | ← | 3 | 1 | 3 | 4 | 6475.6342 | -0.0100 |
| 4 | 0 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 6476.7694 | -0.0152 |
| 4 | 0 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 6477.0892 | -0.0069 |
| 4 | 0 | 4 | 3 | ← | 3 | 1 | 3 | 3 | 6478.5999 | -0.0104 |
| 2 | 1 | 1 | 1 | ← | 1 | 0 | 1 | 0 | 6479.4426 | 0.0144 |
| 2 | 1 | 1 | 2 | ← | 1 | 0 | 1 | 2 | 6480.4117 | 0.0121 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 1 | 1 | 3 | ← | 1 | 0 | 1 | 2 | 6481.0054 | 0.0113 |
| 2 | 1 | 1 | 2 | ← | 1 | 0 | 1 | 1 | 6481.6734 | 0.0094 |
| 2 | 1 | 1 | 1 | ← | 1 | 0 | 1 | 1 | 6482.5996 | 0.0098 |
| 2 | 2 | 1 | 1 | ← | 2 | 1 | 2 | 1 | 6594.2502 | -0.0009 |
| 2 | 2 | 1 | 3 | ← | 2 | 1 | 2 | 3 | 6595.4320 | 0.0050 |
| 2 | 2 | 1 | 1 | ← | 2 | 1 | 2 | 2 | 6595.4320 | -0.0023 |
| 2 | 2 | 0 | 3 | ← | 2 | 1 | 2 | 3 | 6601.5389 | -0.0128 |
| 2 | 2 | 0 | 2 | ← | 2 | 1 | 2 | 3 | 6602.9097 | 0.0000 |
| 2 | 2 | 0 | 2 | ← | 2 | 1 | 2 | 2 | 6603.6548 | -0.0149 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 2 | 6796.9899 | -0.0068 |
| 3 | 2 | 2 | 2 | ← | 3 | 1 | 3 | 2 | 6796.9899 | -0.0072 |
| 3 | 2 | 2 | 4 | ← | 3 | 1 | 3 | 4 | 6797.3933 | -0.0029 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 4 | 6797.3933 | -0.0030 |
| 3 | 2 | 2 | 4 | ← | 3 | 1 | 3 | 3 | 6798.5318 | -0.0050 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 3 | 6798.5318 | -0.0051 |
| 3 | 2 | 2 | 2 | ← | 3 | 1 | 3 | 3 | 6798.5318 | -0.0055 |
| 3 | 2 | 1 | 4 | ← | 3 | 1 | 3 | 4 | 6827.9334 | -0.0006 |
| 3 | 2 | 1 | 3 | ← | 3 | 1 | 3 | 4 | 6827.9334 | -0.0089 |
| 3 | 2 | 1 | 2 | ← | 3 | 1 | 3 | 3 | 6829.0763 | 0.0040 |
| 3 | 2 | 1 | 4 | ← | 3 | 1 | 3 | 3 | 6829.0763 | 0.0016 |
| 4 | 2 | 3 | 3 | ← | 4 | 1 | 4 | 3 | 7068.3005 | -0.0163 |
| 4 | 2 | 3 | 5 | ← | 4 | 1 | 4 | 5 | 7068.4865 | -0.0195 |
| 4 | 2 | 2 | 3 | ← | 4 | 1 | 4 | 3 | 7159.3156 | -0.0028 |
| 4 | 2 | 2 | 5 | ← | 4 | 1 | 4 | 5 | 7159.5071 | -0.0044 |
| 4 | 2 | 2 | 4 | ← | 4 | 1 | 4 | 4 | 7160.2623 | -0.0003 |
| 5 | 0 | 5 | 5 | ← | 4 | 1 | 3 | 4 | 7390.0126 | -0.0163 |
| 5 | 0 | 5 | 6 | ← | 4 | 1 | 3 | 5 | 7390.3690 | -0.0058 |
| 5 | 0 | 5 | 4 | ← | 4 | 1 | 3 | 3 | 7390.3690 | -0.0154 |
| 5 | 2 | 4 | 4 | ← | 5 | 1 | 5 | 4 | 7409.8969 | -0.0001 |
| 5 | 2 | 4 | 6 | ← | 5 | 1 | 5 | 6 | 7410.0065 | 0.0016 |
| 5 | 2 | 4 | 5 | ← | 5 | 1 | 5 | 5 | 7410.5378 | 0.0036 |
| 6 | 2 | 5 | 7 | ← | 6 | 1 | 6 | 7 | 7822.8066 | -0.0177 |
| 3 | 1 | 3 | 3 | ← | 2 | 0 | 2 | 3 | 7963.4147 | 0.0169 |
| 3 | 1 | 3 | 2 | ← | 2 | 0 | 2 | 1 | 7964.1908 | 0.0078 |
| 3 | 1 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 7964.5498 | 0.0114 |
| 3 | 1 | 3 | 3 | ← | 2 | 0 | 2 | 2 | 7964.7653 | 0.0095 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 4 | 8023.7955 | 0.0013 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 8024.9301 | -0.0046 |
| 4 | 1 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 8025.0896 | -0.0163 |
| 4 | 1 | 4 | 3 | ← | 3 | 1 | 3 | 3 | 8026.5855 | 0.0014 |
| 6 | 2 | 4 | 5 | ← | 6 | 1 | 6 | 5 | 8233.4858 | 0.0150 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 4 | 8238.9178 | -0.0074 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 8240.3271 | -0.0114 |
| 4 | 0 | 4 | 3 | ← | 3 | 0 | 3 | 3 | 8242.1592 | -0.0049 |
| 4 | 2 | 3 | 4 | ← | 3 | 2 | 2 | 3 | 8295.6464 | 0.0063 |
| 4 | 2 | 3 | 4 | ← | 3 | 2 | 2 | 4 | 8295.6464 | 0.0062 |
| 4 | 2 | 3 | 5 | ← | 3 | 2 | 2 | 4 | 8296.2173 | 0.0015 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 2 | 8296.3678 | 0.0041 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 3 | 8296.3678 | 0.0037 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 4 | 8296.3678 | 0.0036 |
| 4 | 3 | 1 | 4 | ← | 3 | 3 | 0 | 3 | 8312.6909 | -0.0055 |
| 4 | 3 | 2 | 3 | ← | 3 | 3 | 1 | 2 | 8313.3684 | 0.0006 |
| 4 | 3 | 1 | 5 | ← | 3 | 3 | 0 | 4 | 8313.9359 | -0.0121 |
| 4 | 3 | 1 | 3 | ← | 3 | 3 | 0 | 2 | 8314.4316 | -0.0017 |
| 4 | 2 | 2 | 4 | ← | 3 | 2 | 1 | 3 | 8356.1158 | 0.0011 |
| 4 | 2 | 2 | 4 | ← | 3 | 2 | 1 | 4 | 8356.1158 | -0.0071 |
| 4 | 2 | 2 | 5 | ← | 3 | 2 | 1 | 4 | 8356.6823 | -0.0011 |
| 4 | 1 | 3 | 4 | ← | 3 | 1 | 2 | 4 | 8550.9831 | -0.0059 |
| 4 | 1 | 3 | 4 | ← | 3 | 1 | 2 | 3 | 8551.9738 | 0.0156 |
| 4 | 1 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 8552.1173 | -0.0082 |
| 4 | 1 | 3 | 3 | ← | 3 | 1 | 2 | 3 | 8553.3803 | -0.0068 |
| 5 | 0 | 5 | 5 | ← | 4 | 1 | 4 | 4 | 8709.1213 | -0.0214 |
| 3 | 1 | 2 | 3 | ← | 2 | 0 | 2 | 3 | 8755.5012 | 0.0128 |
| 3 | 1 | 2 | 2 | ← | 2 | 0 | 2 | 1 | 8756.0419 | 0.0000 |
| 3 | 1 | 2 | 4 | ← | 2 | 0 | 2 | 3 | 8756.4723 | 0.0149 |
| 3 | 1 | 2 | 3 | ← | 2 | 0 | 2 | 2 | 8756.8586 | 0.0122 |
| 3 | 1 | 2 | 2 | ← | 2 | 0 | 2 | 2 | 8758.1805 | 0.0254 |

| J' | $K_{a'}$ | $K_{c'}$ | F' | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | 1 | 4 | 3 | ← | 3 | 0 | 3 | 2 | 9788.2514 | 0.0218 |
| 4 | 1 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 9788.3934 | 0.0064 |
| 4 | 1 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 9788.5097 | 0.0211 |
| 4 | 1 | 4 | 3 | ← | 3 | 0 | 3 | 3 | 9790.1463 | 0.0084 |
| 7 | 1 | 6 | 6 | ← | 6 | 2 | 5 | 5 | 9831.3876 | 0.0110 |
| 5 | 1 | 5 | 5 | ← | 4 | 1 | 4 | 5 | 10019.5909 | -0.0055 |
| 5 | 1 | 5 | 6 | ← | 4 | 1 | 4 | 5 | 10021.0111 | 0.0078 |
| 5 | 1 | 5 | 4 | ← | 4 | 1 | 4 | 4 | 10022.5968 | -0.0049 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 5 | 10255.8337 | -0.0072 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 10257.2996 | 0.0067 |
| 5 | 0 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 10257.2996 | -0.0236 |
| 5 | 0 | 5 | 4 | ← | 4 | 0 | 4 | 4 | 10259.0738 | -0.0035 |
| 5 | 2 | 4 | 5 | ← | 4 | 2 | 3 | 4 | 10362.1949 | -0.0050 |
| 5 | 2 | 4 | 6 | ← | 4 | 2 | 3 | 5 | 10362.4888 | -0.0131 |
| 5 | 2 | 4 | 4 | ← | 4 | 2 | 3 | 4 | 10363.2589 | 0.0024 |
| 6 | 3 | 3 | 5 | ← | 6 | 2 | 4 | 5 | 10376.5667 | 0.0019 |
| 5 | 4 | 2 | 5 | ← | 4 | 4 | 1 | 4 | 10388.8294 | -0.0025 |
| 5 | 4 | 2 | 6 | ← | 4 | 4 | 1 | 5 | 10389.9651 | -0.0017 |
| 5 | 3 | 3 | 5 | ← | 4 | 3 | 2 | 4 | 10394.8083 | -0.0038 |
| 5 | 3 | 3 | 6 | ← | 4 | 3 | 2 | 5 | 10395.4640 | 0.0042 |
| 5 | 3 | 3 | 4 | ← | 4 | 3 | 2 | 3 | 10395.5940 | -0.0246 |
| 5 | 3 | 2 | 5 | ← | 4 | 3 | 1 | 4 | 10398.5226 | -0.0085 |
| 5 | 3 | 2 | 6 | ← | 4 | 3 | 1 | 5 | 10399.1709 | -0.0073 |
| 5 | 3 | 2 | 4 | ← | 4 | 3 | 1 | 3 | 10399.3394 | 0.0022 |
| 2 | 2 | 1 | 1 | ← | 1 | 1 | 0 | 1 | 10480.6205 | -0.0028 |
| 5 | 2 | 3 | 5 | ← | 4 | 2 | 2 | 4 | 10480.8818 | 0.0025 |
| 5 | 2 | 3 | 6 | ← | 4 | 2 | 2 | 5 | 10481.1675 | -0.0054 |
| 2 | 2 | 1 | 3 | ← | 1 | 1 | 0 | 2 | 10482.0830 | -0.0021 |
| 2 | 2 | 1 | 1 | ← | 1 | 1 | 0 | 0 | 10482.3931 | -0.0034 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 0 | 1 | 10482.7295 | -0.0012 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 0 | 2 | 10483.4374 | -0.0026 |
| 2 | 2 | 0 | 1 | ← | 1 | 1 | 0 | 1 | 10486.7286 | -0.0177 |
| 2 | 2 | 0 | 3 | ← | 1 | 1 | 0 | 2 | 10488.1986 | -0.0112 |
| 2 | 2 | 0 | 1 | ← | 1 | 1 | 0 | 0 | 10488.5124 | -0.0071 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 0 | 1 | 10488.8443 | -0.0144 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 0 | 2 | 10489.5539 | -0.0139 |
| 5 | 3 | 2 | 4 | ← | 5 | 2 | 3 | 4 | 10511.1793 | -0.0031 |
| 5 | 3 | 2 | 5 | ← | 5 | 2 | 3 | 6 | 10511.1793 | -0.0070 |
| 4 | 3 | 2 | 4 | ← | 4 | 2 | 2 | 4 | 10593.1581 | 0.0130 |
| 2 | 2 | 1 | 1 | ← | 1 | 1 | 1 | 1 | 10612.7757 | -0.0001 |
| 2 | 2 | 1 | 3 | ← | 1 | 1 | 1 | 2 | 10614.0838 | 0.0005 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 1 | 1 | 10614.8759 | -0.0073 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 1 | 2 | 10615.4291 | -0.0089 |
| 2 | 2 | 0 | 1 | ← | 1 | 1 | 1 | 1 | 10618.8957 | -0.0031 |
| 2 | 2 | 0 | 3 | ← | 1 | 1 | 1 | 2 | 10620.2130 | 0.0050 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 1 | 1 | 10621.0067 | -0.0044 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 1 | 2 | 10621.5586 | -0.0073 |
| 5 | 1 | 4 | 5 | ← | 4 | 1 | 3 | 4 | 10677.2853 | -0.0106 |
| 5 | 1 | 4 | 6 | ← | 4 | 1 | 3 | 5 | 10677.3832 | -0.0055 |
| 5 | 1 | 4 | 4 | ← | 4 | 1 | 3 | 4 | 10678.7783 | 0.0024 |
| 6 | 0 | 6 | 6 | ← | 5 | 1 | 5 | 5 | 10938.2025 | -0.0095 |
| 4 | 1 | 3 | 5 | ← | 3 | 0 | 3 | 4 | 11107.3200 | -0.0056 |
| 6 | 1 | 6 | 6 | ← | 5 | 1 | 5 | 5 | 12010.8548 | -0.0051 |
| 6 | 0 | 6 | 6 | ← | 5 | 0 | 5 | 6 | 12248.4889 | -0.0061 |
| 6 | 0 | 6 | 7 | ← | 5 | 0 | 5 | 6 | 12250.0104 | 0.0074 |
| 6 | 0 | 6 | 5 | ← | 5 | 0 | 5 | 5 | 12251.7567 | 0.0166 |
| 6 | 2 | 5 | 6 | ← | 5 | 2 | 4 | 5 | 12423.5629 | 0.0034 |
| 6 | 2 | 5 | 5 | ← | 5 | 2 | 4 | 4 | 12423.7374 | -0.0017 |
| 6 | 2 | 5 | 7 | ← | 5 | 2 | 4 | 6 | 12423.7374 | -0.0020 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 1 | 12424.9883 | -0.0038 |
| 3 | 2 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 12425.3181 | -0.0048 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 1 | 3 | 12425.3181 | -0.0049 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 3 | 12425.3181 | -0.0053 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 12425.9118 | -0.0058 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 2 | 12425.9118 | -0.0062 |
| 3 | 2 | 1 | 2 | ← | 2 | 1 | 1 | 3 | 12455.8670 | 0.0086 |
| 3 | 2 | 1 | 4 | ← | 2 | 1 | 1 | 3 | 12455.8670 | 0.0063 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 2 | 1 | 3 | ← | 2 | 1 | 1 | 3 | 12455.8670 | -0.0019 |
| 3 | 2 | 1 | 2 | ← | 2 | 1 | 1 | 2 | 12456.4611 | 0.0082 |
| 3 | 2 | 1 | 3 | ← | 2 | 1 | 1 | 2 | 12456.4611 | -0.0024 |
| 6 | 3 | 4 | 6 | ← | 5 | 3 | 3 | 5 | 12479.8566 | -0.0070 |
| 6 | 3 | 4 | 7 | ← | 5 | 3 | 3 | 6 | 12480.2441 | 0.0006 |
| 6 | 3 | 3 | 6 | ← | 5 | 3 | 2 | 5 | 12489.7100 | -0.0172 |
| 6 | 3 | 3 | 7 | ← | 5 | 3 | 2 | 6 | 12490.0920 | -0.0142 |
| 6 | 2 | 4 | 6 | ← | 5 | 2 | 3 | 5 | 12624.6105 | -0.0029 |
| 6 | 2 | 4 | 5 | ← | 5 | 2 | 3 | 4 | 12624.7674 | -0.0156 |
| 6 | 2 | 4 | 7 | ← | 5 | 2 | 3 | 6 | 12624.7674 | -0.0166 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 2 | 1 | 12820.9406 | 0.0063 |
| 3 | 2 | 2 | 4 | ← | 2 | 1 | 2 | 3 | 12821.3585 | 0.0015 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 2 | 3 | 12821.3585 | 0.0014 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 2 | 3 | 12821.3585 | 0.0010 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 2 | 2 | 12822.1169 | -0.0001 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 2 | 2 | 12822.1169 | -0.0005 |
| 3 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 1 | 12851.4723 | 0.0030 |
| 3 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 3 | 12851.8890 | -0.0033 |
| 3 | 2 | 1 | 4 | ← | 2 | 1 | 2 | 3 | 12851.8890 | -0.0057 |
| 3 | 2 | 1 | 3 | ← | 2 | 1 | 2 | 3 | 12851.8890 | -0.0140 |
| 3 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 2 | 12852.6576 | 0.0052 |
| 3 | 2 | 1 | 3 | ← | 2 | 1 | 2 | 2 | 12852.6576 | -0.0053 |
| 7 | 0 | 7 | 7 | ← | 6 | 1 | 6 | 6 | 13146.8970 | 0.0064 |
| 6 | 1 | 6 | 7 | ← | 5 | 0 | 5 | 6 | 13322.5935 | -0.0161 |
| 6 | 1 | 6 | 5 | ← | 5 | 0 | 5 | 5 | 13324.3383 | -0.0016 |
| 5 | 1 | 4 | 6 | ← | 4 | 0 | 4 | 5 | 13544.3615 | 0.0243 |
| 5 | 1 | 4 | 5 | ← | 4 | 0 | 4 | 4 | 13544.5832 | 0.0233 |
| 7 | 0 | 7 | 6 | ← | 6 | 0 | 6 | 5 | 14219.5139 | -0.0132 |
| 4 | 2 | 3 | 3 | ← | 3 | 1 | 2 | 2 | 14301.4945 | -0.0072 |
| 4 | 2 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 14301.6932 | 0.0002 |
| 4 | 2 | 3 | 4 | ← | 3 | 1 | 2 | 3 | 14302.0884 | 0.0018 |
| 4 | 2 | 2 | 3 | ← | 3 | 1 | 2 | 2 | 14392.5013 | -0.0020 |
| 4 | 2 | 2 | 5 | ← | 3 | 1 | 2 | 4 | 14392.7022 | 0.0037 |
| 4 | 2 | 2 | 4 | ← | 3 | 1 | 2 | 3 | 14393.1138 | 0.0068 |
| 7 | 5 | 3 | 8 | ← | 6 | 5 | 2 | 7 | 14548.4140 | -0.0073 |
| 7 | 5 | 2 | 8 | ← | 6 | 5 | 1 | 7 | 14548.4140 | -0.0124 |
| 7 | 3 | 5 | 6 | ← | 6 | 3 | 4 | 5 | 14566.8306 | 0.0073 |
| 7 | 3 | 4 | 8 | ← | 6 | 3 | 3 | 7 | 14588.7923 | -0.0018 |
| 7 | 3 | 4 | 6 | ← | 6 | 3 | 3 | 5 | 14588.7923 | -0.0238 |
| 4 | 2 | 3 | 3 | ← | 3 | 1 | 3 | 2 | 15093.3431 | -0.0176 |
| 4 | 2 | 3 | 5 | ← | 3 | 1 | 3 | 4 | 15093.5921 | -0.0198 |
| 4 | 2 | 3 | 4 | ← | 3 | 1 | 3 | 3 | 15094.1612 | -0.0158 |
| 4 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 2 | 15184.3841 | 0.0217 |
| 4 | 2 | 2 | 5 | ← | 3 | 1 | 3 | 4 | 15184.6372 | 0.0197 |
| 4 | 2 | 2 | 4 | ← | 3 | 1 | 3 | 3 | 15185.2135 | 0.0160 |
| 8 | 0 | 8 | 7 | ← | 7 | 1 | 7 | 6 | 15322.7466 | -0.0221 |
| 8 | 1 | 8 | 9 | ← | 7 | 1 | 7 | 8 | 15971.6465 | 0.0139 |
| 8 | 3 | 5 | 7 | ← | 7 | 3 | 4 | 6 | 16697.7803 | 0.0196 |
| 3 | 3 | 1 | 4 | ← | 2 | 2 | 1 | 3 | 16892.3432 | -0.0044 |
| 8 | 2 | 6 | 8 | ← | 7 | 2 | 5 | 7 | 16956.9348 | -0.0233 |
| 9 | 0 | 9 | 8 | ← | 8 | 0 | 8 | 7 | 18108.3991 | 0.0166 |
| 9 | 0 | 9 | 9 | ← | 8 | 0 | 8 | 8 | 18108.3991 | 0.0143 |
| 9 | 0 | 9 | 10 | ← | 8 | 0 | 8 | 9 | 18108.3991 | -0.0033 |
| 9 | 2 | 8 | 8 | ← | 8 | 2 | 7 | 7 | 18567.7726 | 0.0233 |
| 9 | 2 | 8 | 10 | ← | 8 | 2 | 7 | 9 | 18567.7726 | 0.0121 |
| 9 | 1 | 9 | 9 | ← | 8 | 0 | 8 | 8 | 18591.5168 | 0.0222 |
| 9 | 1 | 9 | 10 | ← | 8 | 0 | 8 | 9 | 18591.5168 | 0.0106 |
| 9 | 1 | 9 | 8 | ← | 8 | 0 | 8 | 7 | 18591.5168 | 0.0313 |
| 9 | 8 | 1 | 9 | ← | 8 | 8 | 0 | 9 | 18699.9988 | -0.0174 |
| 9 | 8 | 2 | 9 | ← | 8 | 8 | 1 | 9 | 18699.9988 | -0.0174 |
| 9 | 7 | 2 | 10 | ← | 8 | 7 | 1 | 9 | 18701.8506 | -0.0041 |
| 9 | 7 | 3 | 10 | ← | 8 | 7 | 2 | 9 | 18701.8506 | -0.0041 |
| 9 | 6 | 4 | 9 | ← | 8 | 6 | 3 | 8 | 18707.0808 | 0.0334 |
| 9 | 6 | 3 | 9 | ← | 8 | 6 | 2 | 8 | 18707.0808 | 0.0327 |
| 9 | 6 | 4 | 8 | ← | 8 | 6 | 3 | 7 | 18707.5470 | -0.0079 |
| 9 | 6 | 3 | 8 | ← | 8 | 6 | 2 | 7 | 18707.5470 | -0.0086 |
| 9 | 5 | 5 | 9 | ← | 8 | 5 | 4 | 9 | 18716.8832 | -0.0065 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | 5 | 4 | 9 | ← | 8 | 5 | 3 | 8 | 18716.8832 | -0.0068 |
| 9 | 5 | 4 | 10 | ← | 8 | 5 | 3 | 9 | 18717.2086 | 0.0061 |
| 9 | 5 | 4 | 8 | ← | 8 | 5 | 3 | 9 | 18717.2086 | -0.0215 |
| 9 | 5 | 4 | 8 | ← | 8 | 5 | 3 | 7 | 18717.2086 | -0.0296 |
| 9 | 4 | 6 | 10 | ← | 8 | 4 | 5 | 9 | 18734.2284 | -0.0024 |
| 9 | 4 | 6 | 8 | ← | 8 | 4 | 5 | 7 | 18734.2284 | -0.0180 |
| 9 | 4 | 5 | 10 | ← | 8 | 4 | 4 | 9 | 18737.5586 | -0.0122 |
| 9 | 4 | 5 | 8 | ← | 8 | 4 | 4 | 7 | 18737.5586 | -0.0278 |
| 9 | 3 | 6 | 8 | ← | 8 | 3 | 5 | 7 | 18819.7906 | -0.0086 |
| 9 | 3 | 6 | 10 | ← | 8 | 3 | 5 | 9 | 18819.7906 | -0.0089 |
| 4 | 3 | 2 | 3 | ← | 3 | 2 | 1 | 3 | 18948.5961 | -0.0283 |
| 4 | 3 | 1 | 3 | ← | 3 | 2 | 1 | 3 | 18949.8491 | -0.0186 |
| 4 | 3 | 1 | 3 | ← | 3 | 2 | 1 | 4 | 18949.8491 | -0.0270 |
| 4 | 3 | 1 | 3 | ← | 3 | 2 | 1 | 2 | 18949.8491 | -0.0293 |
| 9 | 1 | 8 | 9 | ← | 8 | 1 | 7 | 8 | 19052.8722 | 0.0207 |
| 9 | 1 | 8 | 8 | ← | 8 | 1 | 7 | 7 | 19052.8722 | 0.0121 |
| 9 | 1 | 8 | 10 | ← | 8 | 1 | 7 | 9 | 19052.8722 | -0.0043 |
| 9 | 2 | 7 | 9 | ← | 8 | 2 | 6 | 9 | 19131.4150 | 0.0022 |
| 9 | 2 | 7 | 9 | ← | 8 | 2 | 6 | 8 | 19132.6370 | 0.0209 |
| 9 | 2 | 7 | 8 | ← | 8 | 2 | 6 | 7 | 19132.6370 | -0.0173 |
| 9 | 2 | 7 | 10 | ← | 8 | 2 | 6 | 9 | 19132.6370 | -0.0288 |
| 7 | 2 | 6 | 8 | ← | 6 | 1 | 5 | 7 | 19544.2047 | 0.0099 |
| 10 | 0 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 19556.7603 | -0.0155 |
| 10 | 0 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 19556.7603 | -0.0218 |
| 6 | 2 | 5 | 6 | ← | 5 | 1 | 5 | 5 | 19834.1093 | 0.0158 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 10 | 19906.4970 | -0.0112 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 19908.0821 | 0.0118 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 19908.0821 | 0.0089 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 19908.0821 | -0.0068 |
| 11 | 1 | 10 | 11 | ← | 10 | 2 | 9 | 10 | 19911.7852 | -0.0126 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 20039.8971 | 0.0118 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 20039.8971 | 0.0114 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 20039.8971 | -0.0043 |
| 6 | 2 | 4 | 7 | ← | 5 | 1 | 5 | 6 | 20244.4861 | 0.0207 |
| 6 | 2 | 4 | 6 | ← | 5 | 1 | 5 | 5 | 20244.8531 | 0.0058 |
| 10 | 1 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 20391.1926 | 0.0162 |
| 10 | 1 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 20391.1926 | 0.0124 |
| 10 | 1 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 20391.1926 | -0.0001 |
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 8 | 20599.8844 | 0.0233 |
| 10 | 2 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 20599.8844 | 0.0130 |
| 10 | 7 | 4 | 10 | ← | 9 | 7 | 3 | 9 | 20783.3380 | 0.0250 |
| 10 | 7 | 4 | 9 | ← | 9 | 7 | 3 | 8 | 20783.8240 | 0.0113 |
| 10 | 7 | 3 | 9 | ← | 9 | 7 | 2 | 8 | 20783.8240 | 0.0112 |
| 10 | 6 | 5 | 10 | ← | 9 | 6 | 4 | 9 | 20791.2498 | 0.0282 |
| 10 | 6 | 4 | 10 | ← | 9 | 6 | 3 | 9 | 20791.2498 | 0.0257 |
| 10 | 6 | 5 | 9 | ← | 9 | 6 | 4 | 8 | 20791.5929 | 0.0070 |
| 10 | 6 | 4 | 9 | ← | 9 | 6 | 3 | 8 | 20791.5929 | 0.0044 |
| 10 | 5 | 6 | 10 | ← | 9 | 5 | 5 | 9 | 20804.5687 | -0.0020 |
| 10 | 5 | 5 | 9 | ← | 9 | 5 | 4 | 10 | 20805.0167 | -0.0162 |
| 10 | 5 | 5 | 9 | ← | 9 | 5 | 4 | 8 | 20805.0167 | 0.0114 |
| 10 | 4 | 7 | 11 | ← | 9 | 4 | 6 | 10 | 20827.1912 | -0.0123 |
| 10 | 4 | 7 | 9 | ← | 9 | 4 | 6 | 8 | 20827.1912 | -0.0194 |
| 10 | 4 | 6 | 11 | ← | 9 | 4 | 5 | 10 | 20834.3657 | -0.0129 |
| 10 | 4 | 6 | 9 | ← | 9 | 4 | 5 | 8 | 20834.3657 | -0.0199 |
| 10 | 3 | 7 | 9 | ← | 9 | 3 | 6 | 8 | 20957.6904 | 0.0129 |
| 10 | 3 | 7 | 11 | ← | 9 | 3 | 6 | 10 | 20957.6904 | 0.0096 |
| 5 | 3 | 3 | 5 | ← | 4 | 2 | 2 | 5 | 20987.4259 | 0.0292 |
| 5 | 3 | 3 | 4 | ← | 4 | 2 | 2 | 3 | 20987.4259 | 0.0025 |
| 5 | 3 | 2 | 4 | ← | 4 | 2 | 2 | 3 | 20992.3905 | 0.0052 |
| 5 | 3 | 3 | 4 | ← | 4 | 2 | 3 | 3 | 21078.4283 | 0.0032 |
| 5 | 3 | 3 | 5 | ← | 4 | 2 | 3 | 5 | 21078.4283 | 0.0261 |
| 5 | 3 | 2 | 4 | ← | 4 | 2 | 3 | 3 | 21083.3942 | 0.0073 |
| 10 | 1 | 9 | 10 | ← | 9 | 1 | 8 | 9 | 21098.5425 | 0.0209 |
| 10 | 1 | 9 | 9 | ← | 9 | 1 | 8 | 8 | 21098.5425 | 0.0129 |
| 10 | 1 | 9 | 11 | ← | 9 | 1 | 8 | 10 | 21098.5425 | -0.0005 |
| 8 | 2 | 7 | 9 | ← | 7 | 1 | 6 | 8 | 21174.8278 | 0.0134 |
| 10 | 2 | 8 | 10 | ← | 9 | 2 | 7 | 9 | 21304.5178 | -0.0031 |

| J’ | $K_{a'}$ | $K_{c'}$ | F’ | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | 2 | 8 | 9 | ← | 9 | 2 | 7 | 8 | 21304.5178 | -0.0289 |
| 11 | 0 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 21618.1012 | 0.0001 |
| 11 | 0 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 21618.1012 | -0.0038 |
| 11 | 0 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 21618.1012 | -0.0168 |
| 11 | 1 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 21868.5774 | 0.0065 |
| 11 | 1 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 21868.5774 | 0.0042 |
| 11 | 1 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 21868.5774 | -0.0087 |
| 11 | 0 | 11 | 11 | ← | 10 | 0 | 10 | 10 | 21969.4004 | 0.0049 |
| 11 | 0 | 11 | 10 | ← | 10 | 0 | 10 | 9 | 21969.4004 | 0.0044 |
| 11 | 0 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 21969.4004 | -0.0089 |
| 11 | 1 | 11 | 10 | ← | 10 | 0 | 10 | 9 | 22219.8821 | 0.0179 |
| 11 | 1 | 11 | 11 | ← | 10 | 0 | 10 | 10 | 22219.8821 | 0.0167 |
| 11 | 1 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 22219.8821 | 0.0045 |
| 8 | 2 | 6 | 8 | ← | 7 | 1 | 6 | 8 | 22320.4302 | 0.0041 |
| 8 | 2 | 6 | 9 | ← | 7 | 1 | 6 | 8 | 22321.6301 | 0.0007 |
| 11 | 2 | 10 | 10 | ← | 10 | 2 | 9 | 9 | 22623.0726 | 0.0273 |
| 11 | 2 | 10 | 12 | ← | 10 | 2 | 9 | 11 | 22623.0726 | 0.0180 |
| 9 | 2 | 8 | 9 | ← | 8 | 1 | 7 | 8 | 22758.2511 | 0.0095 |
| 11 | 7 | 5 | 10 | ← | 10 | 7 | 4 | 9 | 22866.9647 | -0.0046 |
| 11 | 6 | 5 | 11 | ← | 10 | 6 | 4 | 10 | 22877.1145 | -0.0026 |
| 11 | 6 | 6 | 10 | ← | 10 | 6 | 5 | 9 | 22877.4059 | 0.0269 |
| 11 | 6 | 6 | 10 | ← | 10 | 6 | 5 | 11 | 22877.4059 | 0.0243 |
| 11 | 6 | 5 | 10 | ← | 10 | 6 | 4 | 9 | 22877.4059 | 0.0186 |
| 11 | 5 | 7 | 12 | ← | 10 | 5 | 6 | 11 | 22894.9690 | -0.0073 |
| 11 | 5 | 7 | 10 | ← | 10 | 5 | 6 | 9 | 22894.9690 | -0.0187 |
| 11 | 3 | 9 | 10 | ← | 10 | 3 | 8 | 9 | 22911.7035 | 0.0237 |
| 11 | 3 | 9 | 12 | ← | 10 | 3 | 8 | 11 | 22911.7035 | 0.0192 |
| 11 | 4 | 8 | 12 | ← | 10 | 4 | 7 | 11 | 22922.9336 | 0.0060 |
| 11 | 4 | 8 | 10 | ← | 10 | 4 | 7 | 9 | 22922.9336 | 0.0035 |
| 11 | 4 | 7 | 12 | ← | 10 | 4 | 6 | 11 | 22937.1086 | -0.0025 |
| 11 | 4 | 7 | 10 | ← | 10 | 4 | 6 | 9 | 22937.1086 | -0.0049 |
| 7 | 2 | 5 | 7 | ← | 6 | 1 | 6 | 6 | 23019.1069 | -0.0155 |
| 11 | 3 | 8 | 11 | ← | 10 | 3 | 7 | 10 | 23113.3879 | 0.0234 |
| 11 | 3 | 8 | 10 | ← | 10 | 3 | 7 | 9 | 23113.3879 | -0.0332 |
| 11 | 1 | 10 | 11 | ← | 10 | 1 | 9 | 10 | 23118.5146 | 0.0221 |
| 11 | 1 | 10 | 10 | ← | 10 | 1 | 9 | 9 | 23118.5146 | 0.0142 |
| 11 | 1 | 10 | 12 | ← | 10 | 1 | 9 | 11 | 23118.5146 | 0.0030 |
| 6 | 3 | 4 | 5 | ← | 5 | 2 | 4 | 4 | 23196.1963 | 0.0012 |
| 6 | 3 | 3 | 5 | ← | 5 | 2 | 4 | 4 | 23211.0234 | 0.0038 |
| 11 | 2 | 9 | 11 | ← | 10 | 2 | 8 | 10 | 23466.2685 | -0.0185 |
| 12 | 1 | 12 | 12 | ← | 11 | 1 | 11 | 11 | 23824.8994 | -0.0031 |
| 12 | 1 | 12 | 11 | ← | 11 | 1 | 11 | 10 | 23824.8994 | -0.0049 |
| 12 | 1 | 12 | 13 | ← | 11 | 1 | 11 | 12 | 23824.8994 | -0.0162 |
| 12 | 0 | 12 | 12 | ← | 11 | 0 | 11 | 11 | 23899.6578 | -0.0023 |
| 12 | 0 | 12 | 11 | ← | 11 | 0 | 11 | 10 | 23899.6578 | -0.0033 |
| 12 | 0 | 12 | 13 | ← | 11 | 0 | 11 | 12 | 23899.6578 | -0.0145 |
| 12 | 1 | 12 | 12 | ← | 11 | 0 | 11 | 11 | 24075.3767 | 0.0043 |
| 12 | 1 | 12 | 11 | ← | 11 | 0 | 11 | 10 | 24075.3767 | 0.0041 |
| 12 | 1 | 12 | 13 | ← | 11 | 0 | 11 | 12 | 24075.3767 | -0.0071 |
| 12 | 2 | 11 | 13 | ← | 11 | 2 | 10 | 12 | 24637.0471 | 0.0322 |
| 8 | 2 | 7 | 9 | ← | 7 | 1 | 7 | 8 | 24834.5550 | 0.0281 |
| 12 | 7 | 6 | 13 | ← | 11 | 7 | 5 | 12 | 24951.4873 | -0.0214 |
| 12 | 7 | 5 | 13 | ← | 11 | 7 | 4 | 12 | 24951.4873 | -0.0217 |
| 12 | 6 | 7 | 13 | ← | 11 | 6 | 6 | 12 | 24965.1069 | 0.0152 |
| 12 | 6 | 7 | 11 | ← | 11 | 6 | 6 | 10 | 24965.1069 | 0.0013 |
| 12 | 6 | 6 | 13 | ← | 11 | 6 | 5 | 12 | 24965.1069 | -0.0080 |
| 12 | 6 | 6 | 11 | ← | 11 | 6 | 5 | 10 | 24965.1069 | -0.0219 |
| 12 | 6 | 7 | 11 | ← | 11 | 6 | 6 | 12 | 24965.1069 | -0.0235 |
| 12 | 5 | 7 | 13 | ← | 11 | 5 | 6 | 12 | 24988.9131 | -0.0043 |
| 12 | 5 | 7 | 11 | ← | 11 | 5 | 6 | 10 | 24988.9131 | -0.0106 |
| 12 | 3 | 10 | 11 | ← | 11 | 3 | 9 | 10 | 24990.9459 | 0.0014 |
| 12 | 3 | 10 | 13 | ← | 11 | 3 | 9 | 12 | 24990.9459 | -0.0033 |
| 12 | 4 | 9 | 11 | ← | 11 | 4 | 8 | 10 | 25021.0955 | 0.0240 |
| 12 | 4 | 9 | 13 | ← | 11 | 4 | 8 | 12 | 25021.0955 | 0.0239 |
| 12 | 4 | 8 | 11 | ← | 11 | 4 | 7 | 10 | 25047.2560 | 0.0022 |
| 12 | 4 | 8 | 13 | ← | 11 | 4 | 7 | 12 | 25047.2560 | 0.0021 |
| 12 | 1 | 11 | 13 | ← | 11 | 1 | 10 | 12 | 25111.5022 | 0.0063 |

| J' | $K_{a'}$ | $K_{c'}$ | F' | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | 4 | 1 | 6 | ← | 4 | 3 | 1 | 5 | 25306.0222 | -0.0064 |
| 5 | 4 | 2 | 4 | ← | 4 | 3 | 2 | 4 | 25306.5783 | 0.0289 |
| 13 | 1 | 13 | 13 | ← | 12 | 1 | 12 | 12 | 25777.8112 | -0.0171 |
| 13 | 1 | 13 | 12 | ← | 12 | 1 | 12 | 11 | 25777.8112 | -0.0187 |
| 13 | 1 | 13 | 14 | ← | 12 | 1 | 12 | 13 | 25777.8112 | -0.0282 |
| 13 | 0 | 13 | 13 | ← | 12 | 0 | 12 | 12 | 25831.8963 | -0.0139 |
| 13 | 0 | 13 | 12 | ← | 12 | 0 | 12 | 11 | 25831.8963 | -0.0151 |
| 13 | 0 | 13 | 14 | ← | 12 | 0 | 12 | 13 | 25831.8963 | -0.0247 |
| | | | | | | | | | RMS | 11.4 kHz |

Table S11 Linelist for Conformer III of isoleucinol. OMC is the difference between the observed and calculated transition.

| J' | $K_{a'}$ | $K_{c'}$ | F' | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 1 | 1 | ← | 0 | 0 | 0 | 1 | 2223.1004 | -0.0012 |
| 1 | 0 | 1 | 2 | ← | 0 | 0 | 0 | 1 | 2224.1474 | -0.0010 |
| 1 | 0 | 1 | 0 | ← | 0 | 0 | 0 | 1 | 2225.7179 | -0.0009 |
| 1 | 1 | 1 | 0 | ← | 0 | 0 | 0 | 1 | 4077.1309 | 0.0076 |
| 1 | 1 | 1 | 2 | ← | 0 | 0 | 0 | 1 | 4078.0108 | -0.0049 |
| 2 | 1 | 2 | 2 | ← | 1 | 1 | 1 | 1 | 4244.2099 | 0.0127 |
| 2 | 1 | 2 | 2 | ← | 1 | 1 | 1 | 2 | 4244.8046 | 0.0124 |
| 2 | 1 | 2 | 1 | ← | 1 | 1 | 1 | 1 | 4244.9591 | 0.0084 |
| 2 | 1 | 2 | 3 | ← | 1 | 1 | 1 | 2 | 4245.2835 | 0.0074 |
| 2 | 1 | 2 | 1 | ← | 1 | 1 | 1 | 0 | 4246.4466 | 0.0085 |
| 1 | 1 | 0 | 0 | ← | 0 | 0 | 0 | 1 | 4280.2434 | 0.0043 |
| 1 | 1 | 0 | 2 | ← | 0 | 0 | 0 | 1 | 4280.9227 | 0.0061 |
| 1 | 1 | 0 | 1 | ← | 0 | 0 | 0 | 1 | 4281.3850 | 0.0169 |
| 3 | 0 | 3 | 3 | ← | 2 | 1 | 1 | 2 | 4333.5134 | -0.0043 |
| 3 | 0 | 3 | 4 | ← | 2 | 1 | 1 | 3 | 4334.0093 | -0.0024 |
| 5 | 2 | 4 | 4 | ← | 5 | 1 | 4 | 4 | 4419.1846 | 0.0123 |
| 5 | 2 | 4 | 6 | ← | 5 | 1 | 4 | 6 | 4419.2660 | 0.0059 |
| 5 | 2 | 4 | 5 | ← | 5 | 1 | 4 | 5 | 4419.6978 | 0.0065 |
| 2 | 0 | 2 | 2 | ← | 1 | 0 | 1 | 2 | 4431.1554 | 0.0010 |
| 2 | 0 | 2 | 1 | ← | 1 | 0 | 1 | 0 | 4431.3190 | 0.0094 |
| 2 | 0 | 2 | 2 | ← | 1 | 0 | 1 | 1 | 4432.1949 | -0.0061 |
| 2 | 0 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 4432.2665 | 0.0030 |
| 2 | 0 | 2 | 1 | ← | 1 | 0 | 1 | 1 | 4433.9286 | 0.0018 |
| 2 | 1 | 1 | 2 | ← | 1 | 1 | 0 | 1 | 4649.9594 | 0.0093 |
| 2 | 1 | 1 | 2 | ← | 1 | 1 | 0 | 2 | 4650.4051 | 0.0036 |
| 2 | 1 | 1 | 1 | ← | 1 | 1 | 0 | 1 | 4650.9373 | -0.0049 |
| 2 | 1 | 1 | 3 | ← | 1 | 1 | 0 | 2 | 4651.0436 | 0.0046 |
| 2 | 1 | 1 | 1 | ← | 1 | 1 | 0 | 0 | 4652.0713 | 0.0000 |
| 4 | 2 | 3 | 3 | ← | 4 | 1 | 3 | 3 | 4883.9675 | 0.0083 |
| 4 | 2 | 3 | 5 | ← | 4 | 1 | 3 | 5 | 4884.1149 | -0.0005 |
| 4 | 2 | 3 | 4 | ← | 4 | 1 | 3 | 4 | 4884.7274 | 0.0035 |
| 3 | 0 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 4942.0315 | 0.0036 |
| 3 | 0 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 4942.6699 | -0.0055 |
| 4 | 2 | 2 | 3 | ← | 4 | 1 | 3 | 3 | 5114.2243 | 0.0019 |
| 4 | 2 | 2 | 5 | ← | 4 | 1 | 3 | 5 | 5114.3667 | 0.0022 |
| 4 | 2 | 2 | 4 | ← | 4 | 1 | 3 | 4 | 5114.9217 | 0.0048 |
| 6 | 1 | 6 | 6 | ← | 5 | 2 | 4 | 5 | 5187.4640 | -0.0048 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 2 | 2 | 5267.8080 | 0.0019 |
| 3 | 2 | 2 | 2 | ← | 3 | 1 | 2 | 2 | 5267.8080 | 0.0016 |
| 3 | 2 | 2 | 4 | ← | 3 | 1 | 2 | 4 | 5268.1396 | 0.0016 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 2 | 4 | 5268.1396 | 0.0015 |
| 3 | 2 | 2 | 4 | ← | 3 | 1 | 2 | 3 | 5269.0824 | -0.0031 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 2 | 3 | 5269.0824 | -0.0032 |
| 3 | 2 | 2 | 2 | ← | 3 | 1 | 2 | 3 | 5269.0824 | -0.0035 |
| 3 | 2 | 1 | 4 | ← | 3 | 1 | 2 | 4 | 5346.2829 | -0.0077 |
| 3 | 2 | 1 | 3 | ← | 3 | 1 | 2 | 3 | 5347.2082 | 0.0015 |
| 7 | 2 | 6 | 7 | ← | 6 | 3 | 4 | 6 | 5398.1920 | 0.0094 |
| 2 | 2 | 1 | 1 | ← | 2 | 1 | 1 | 1 | 5561.0540 | -0.0036 |
| 2 | 2 | 1 | 3 | ← | 2 | 1 | 1 | 3 | 5562.0346 | -0.0008 |
| 2 | 2 | 1 | 1 | ← | 2 | 1 | 1 | 2 | 5562.0346 | -0.0153 |
| 2 | 2 | 1 | 2 | ← | 2 | 1 | 1 | 2 | 5563.7959 | 0.0013 |
| 7 | 1 | 7 | 6 | ← | 6 | 2 | 4 | 5 | 5619.5737 | -0.0044 |
| 2 | 1 | 2 | 1 | ← | 1 | 0 | 1 | 0 | 6097.8559 | 0.0133 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 1 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 6099.1436 | 0.0001 |
| 4 | 0 | 4 | 4 | ← | 3 | 1 | 2 | 3 | 6111.5224 | -0.0081 |
| 4 | 0 | 4 | 5 | ← | 3 | 1 | 2 | 4 | 6111.7077 | -0.0088 |
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 3 | 6357.4114 | 0.0028 |
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 6357.8917 | -0.0008 |
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 6358.1978 | 0.0003 |
| 3 | 1 | 3 | 2 | ← | 2 | 1 | 2 | 1 | 6358.1978 | -0.0066 |
| 3 | 1 | 3 | 2 | ← | 2 | 1 | 2 | 2 | 6358.9585 | 0.0006 |
| 5 | 1 | 4 | 5 | ← | 4 | 2 | 2 | 4 | 6434.7693 | -0.0092 |
| 5 | 1 | 4 | 6 | ← | 4 | 2 | 2 | 5 | 6435.3895 | -0.0084 |
| 5 | 1 | 4 | 4 | ← | 4 | 2 | 2 | 3 | 6435.4876 | -0.0080 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 4 | 6484.6578 | -0.0084 |
| 3 | 2 | 2 | 4 | ← | 3 | 1 | 3 | 4 | 6484.6578 | -0.0084 |
| 3 | 2 | 2 | 4 | ← | 3 | 1 | 3 | 3 | 6485.4495 | -0.0055 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 3 | 6485.4495 | -0.0056 |
| 3 | 2 | 2 | 2 | ← | 3 | 1 | 3 | 3 | 6485.4495 | -0.0059 |
| 3 | 2 | 1 | 4 | ← | 3 | 1 | 3 | 4 | 6562.8197 | 0.0008 |
| 3 | 2 | 1 | 3 | ← | 3 | 1 | 3 | 3 | 6563.5639 | -0.0122 |
| 3 | 0 | 3 | 3 | ← | 2 | 0 | 2 | 3 | 6608.4203 | -0.0036 |
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 1 | 6609.3339 | -0.0012 |
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 6609.5688 | 0.0132 |
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 2 | 6611.0743 | 0.0134 |
| 5 | 1 | 4 | 5 | ← | 4 | 2 | 3 | 4 | 6664.9687 | -0.0029 |
| 5 | 1 | 4 | 6 | ← | 4 | 2 | 3 | 5 | 6665.6409 | -0.0059 |
| 3 | 2 | 2 | 3 | ← | 2 | 2 | 1 | 2 | 6671.0436 | 0.0005 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 2 | 6671.0436 | 0.0002 |
| 3 | 2 | 2 | 3 | ← | 2 | 2 | 1 | 3 | 6672.1634 | -0.0012 |
| 3 | 2 | 2 | 4 | ← | 2 | 2 | 1 | 3 | 6672.1634 | -0.0011 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 3 | 6672.1634 | -0.0015 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 1 | 6672.7903 | 0.0022 |
| 2 | 1 | 1 | 1 | ← | 1 | 0 | 1 | 0 | 6706.5946 | 0.0031 |
| 2 | 1 | 1 | 2 | ← | 1 | 0 | 1 | 2 | 6707.1696 | 0.0000 |
| 2 | 1 | 1 | 3 | ← | 1 | 0 | 1 | 2 | 6707.8158 | 0.0085 |
| 2 | 1 | 1 | 2 | ← | 1 | 0 | 1 | 1 | 6708.2217 | 0.0053 |
| 2 | 1 | 1 | 1 | ← | 1 | 0 | 1 | 1 | 6709.2159 | 0.0072 |
| 3 | 2 | 1 | 3 | ← | 2 | 2 | 0 | 2 | 6733.4239 | 0.0035 |
| 3 | 2 | 1 | 4 | ← | 2 | 2 | 0 | 3 | 6734.5676 | 0.0066 |
| 3 | 2 | 1 | 2 | ← | 2 | 2 | 0 | 1 | 6735.1928 | 0.0042 |
| 4 | 2 | 3 | 4 | ← | 4 | 1 | 4 | 5 | 6907.0734 | -0.0119 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 3 | 6965.1260 | 0.0116 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 6965.7606 | 0.0086 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6966.0756 | 0.0135 |
| 3 | 1 | 2 | 2 | ← | 2 | 1 | 1 | 2 | 6967.0383 | 0.0067 |
| 4 | 2 | 2 | 3 | ← | 4 | 1 | 4 | 3 | 7137.6947 | -0.0115 |
| 4 | 2 | 2 | 5 | ← | 4 | 1 | 4 | 5 | 7137.8171 | 0.0101 |
| 4 | 2 | 2 | 4 | ← | 4 | 1 | 4 | 4 | 7138.1970 | -0.0017 |
| 4 | 0 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 7327.8904 | -0.0095 |
| 4 | 0 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 7328.2369 | -0.0079 |
| 5 | 0 | 5 | 4 | ← | 4 | 1 | 3 | 3 | 7673.8061 | -0.0020 |
| 5 | 0 | 5 | 5 | ← | 4 | 1 | 3 | 4 | 7673.8061 | -0.0058 |
| 3 | 2 | 2 | 3 | ← | 3 | 0 | 3 | 2 | 7899.7971 | 0.0050 |
| 3 | 2 | 2 | 2 | ← | 3 | 0 | 3 | 2 | 7899.7971 | 0.0046 |
| 3 | 2 | 2 | 4 | ← | 3 | 0 | 3 | 4 | 7900.1958 | 0.0075 |
| 3 | 2 | 2 | 3 | ← | 3 | 0 | 3 | 4 | 7900.1958 | 0.0075 |
| 3 | 2 | 2 | 3 | ← | 3 | 0 | 3 | 3 | 7901.3225 | 0.0026 |
| 3 | 2 | 2 | 4 | ← | 3 | 0 | 3 | 3 | 7901.3225 | 0.0027 |
| 3 | 2 | 2 | 2 | ← | 3 | 0 | 3 | 3 | 7901.3225 | 0.0023 |
| 3 | 1 | 3 | 3 | ← | 2 | 0 | 2 | 2 | 8025.4078 | 0.0099 |
| 4 | 2 | 3 | 5 | ← | 4 | 0 | 4 | 5 | 8040.1688 | 0.0177 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 4 | 8459.9234 | 0.0058 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 8460.7184 | 0.0119 |
| 4 | 1 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 8460.8316 | -0.0062 |
| 4 | 1 | 4 | 3 | ← | 3 | 1 | 3 | 3 | 8461.8620 | -0.0016 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 4 | 8742.6311 | -0.0020 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 8743.7709 | 0.0062 |
| 4 | 0 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 8743.7709 | 0.0040 |
| 4 | 0 | 4 | 3 | ← | 3 | 0 | 3 | 3 | 8745.1889 | -0.0012 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | 1 | 5 | 6 | ← | 5 | 2 | 3 | 5 | 8864.7565 | -0.0122 |
| 4 | 2 | 3 | 4 | ← | 3 | 2 | 2 | 3 | 8883.2715 | 0.0146 |
| 4 | 2 | 3 | 4 | ← | 3 | 2 | 2 | 4 | 8883.2715 | 0.0145 |
| 4 | 2 | 3 | 5 | ← | 3 | 2 | 2 | 4 | 8883.7516 | 0.0219 |
| 4 | 3 | 2 | 4 | ← | 3 | 3 | 1 | 3 | 8924.4335 | 0.0086 |
| 4 | 3 | 1 | 4 | ← | 3 | 3 | 0 | 3 | 8929.0307 | 0.0215 |
| 4 | 3 | 1 | 5 | ← | 3 | 3 | 0 | 4 | 8930.0768 | 0.0227 |
| 4 | 3 | 1 | 3 | ← | 3 | 3 | 0 | 2 | 8930.4735 | 0.0159 |
| 4 | 3 | 1 | 4 | ← | 3 | 3 | 0 | 4 | 8930.4735 | 0.0146 |
| 6 | 0 | 6 | 5 | ← | 5 | 1 | 4 | 4 | 8997.5524 | -0.0251 |
| 4 | 2 | 2 | 4 | ← | 3 | 2 | 1 | 3 | 9035.3324 | 0.0034 |
| 4 | 2 | 2 | 5 | ← | 3 | 2 | 1 | 4 | 9035.8350 | 0.0090 |
| 3 | 1 | 2 | 3 | ← | 2 | 0 | 2 | 3 | 9240.6637 | 0.0055 |
| 3 | 1 | 2 | 2 | ← | 2 | 0 | 2 | 1 | 9241.3268 | 0.0056 |
| 3 | 1 | 2 | 3 | ← | 2 | 0 | 2 | 2 | 9241.7738 | 0.0065 |
| 3 | 1 | 2 | 2 | ← | 2 | 0 | 2 | 2 | 9243.0618 | 0.0149 |
| 4 | 1 | 3 | 4 | ← | 3 | 1 | 2 | 4 | 9266.6666 | -0.0044 |
| 4 | 1 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 9267.7311 | -0.0210 |
| 4 | 1 | 3 | 3 | ← | 3 | 1 | 2 | 3 | 9268.9812 | 0.0032 |
| 6 | 3 | 3 | 5 | ← | 6 | 2 | 5 | 5 | 10110.7403 | -0.0257 |
| 2 | 2 | 1 | 1 | ← | 1 | 1 | 0 | 1 | 10211.9892 | -0.0106 |
| 2 | 2 | 1 | 3 | ← | 1 | 1 | 0 | 2 | 10213.0721 | -0.0023 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 0 | 1 | 10213.7459 | 0.0013 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 0 | 2 | 10214.2023 | 0.0063 |
| 2 | 2 | 0 | 1 | ← | 1 | 1 | 0 | 1 | 10227.7583 | -0.0047 |
| 2 | 2 | 0 | 3 | ← | 1 | 1 | 0 | 2 | 10228.8321 | 0.0014 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 0 | 1 | 10229.4841 | -0.0041 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 0 | 2 | 10229.9347 | -0.0050 |
| 2 | 2 | 1 | 3 | ← | 1 | 1 | 1 | 2 | 10415.9750 | -0.0002 |
| 2 | 2 | 1 | 1 | ← | 1 | 1 | 1 | 0 | 10416.2420 | -0.0026 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 1 | 1 | 10416.4983 | -0.0035 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 1 | 2 | 10417.0942 | -0.0025 |
| 2 | 2 | 0 | 3 | ← | 1 | 1 | 1 | 2 | 10431.7278 | -0.0035 |
| 2 | 2 | 0 | 1 | ← | 1 | 1 | 1 | 0 | 10432.0293 | 0.0214 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 1 | 1 | 10432.2323 | -0.0132 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 1 | 2 | 10432.8524 | 0.0118 |
| 5 | 1 | 5 | 5 | ← | 4 | 1 | 4 | 5 | 10550.3334 | 0.0069 |
| 5 | 1 | 5 | 4 | ← | 4 | 1 | 4 | 3 | 10551.2993 | 0.0196 |
| 5 | 1 | 5 | 6 | ← | 4 | 1 | 4 | 5 | 10551.2993 | -0.0157 |
| 5 | 1 | 5 | 4 | ← | 4 | 1 | 4 | 4 | 10552.4384 | 0.0016 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 5 | 10828.7714 | 0.0047 |
| 5 | 0 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 10829.8928 | 0.0003 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 10829.8928 | -0.0075 |
| 5 | 0 | 5 | 4 | ← | 4 | 0 | 4 | 4 | 10831.2640 | 0.0084 |
| 5 | 2 | 4 | 5 | ← | 4 | 2 | 3 | 4 | 11084.6725 | 0.0095 |
| 5 | 2 | 4 | 6 | ← | 4 | 2 | 3 | 5 | 11084.9212 | 0.0143 |
| 5 | 3 | 3 | 5 | ← | 4 | 3 | 2 | 4 | 11165.9762 | -0.0018 |
| 5 | 3 | 3 | 6 | ← | 4 | 3 | 2 | 5 | 11166.5141 | -0.0051 |
| 5 | 3 | 3 | 4 | ← | 4 | 3 | 2 | 3 | 11166.6414 | -0.0097 |
| 5 | 3 | 2 | 5 | ← | 4 | 3 | 1 | 4 | 11181.8850 | -0.0060 |
| 5 | 3 | 2 | 6 | ← | 4 | 3 | 1 | 5 | 11182.4303 | -0.0058 |
| 5 | 2 | 3 | 5 | ← | 4 | 2 | 2 | 5 | 11373.7846 | -0.0163 |
| 5 | 2 | 3 | 5 | ← | 4 | 2 | 2 | 4 | 11374.3180 | -0.0115 |
| 5 | 2 | 3 | 6 | ← | 4 | 2 | 2 | 5 | 11374.5906 | -0.0089 |
| 5 | 2 | 3 | 4 | ← | 4 | 2 | 2 | 4 | 11375.2900 | -0.0009 |
| 5 | 1 | 4 | 5 | ← | 4 | 1 | 3 | 5 | 11548.6094 | -0.0050 |
| 5 | 1 | 4 | 5 | ← | 4 | 1 | 3 | 4 | 11549.7162 | 0.0207 |
| 5 | 1 | 4 | 4 | ← | 4 | 1 | 3 | 3 | 11549.7162 | -0.0018 |
| 5 | 1 | 4 | 4 | ← | 4 | 1 | 3 | 4 | 11551.0767 | -0.0005 |
| 6 | 0 | 6 | 5 | ← | 5 | 1 | 5 | 4 | 12019.5019 | 0.0020 |
| 6 | 0 | 6 | 7 | ← | 5 | 1 | 5 | 6 | 12019.5019 | -0.0110 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 1 | 3 | 12234.2050 | 0.0049 |
| 3 | 2 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 12234.2050 | 0.0050 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 3 | 12234.2050 | 0.0046 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 12234.8355 | -0.0021 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 2 | 12234.8355 | -0.0024 |
| 3 | 2 | 1 | 4 | ← | 2 | 1 | 1 | 3 | 12312.3464 | -0.0061 |

| J’ | $K_{a'}$ | $K_{c'}$ | F’ | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 2 | 1 | 2 | ← | 2 | 1 | 1 | 3 | 12312.3464 | -0.0176 |
| 3 | 2 | 1 | 3 | ← | 2 | 1 | 1 | 2 | 12312.9495 | -0.0090 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 2 | 1 | 12842.5918 | -0.0027 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 2 | 3 | 12842.8704 | 0.0066 |
| 3 | 2 | 2 | 4 | ← | 2 | 1 | 2 | 3 | 12842.8704 | 0.0067 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 2 | 3 | 12842.8704 | 0.0063 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 2 | 2 | 12843.3535 | 0.0058 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 2 | 2 | 12843.3535 | 0.0055 |
| 6 | 0 | 6 | 7 | ← | 5 | 0 | 5 | 6 | 12873.5241 | -0.0044 |
| 6 | 0 | 6 | 6 | ← | 5 | 0 | 5 | 5 | 12873.5241 | -0.0154 |
| 3 | 2 | 1 | 3 | ← | 2 | 1 | 2 | 3 | 12920.9949 | 0.0101 |
| 6 | 2 | 5 | 5 | ← | 5 | 2 | 4 | 4 | 13273.1916 | -0.0219 |
| 6 | 2 | 5 | 7 | ← | 5 | 2 | 4 | 6 | 13273.1916 | -0.0231 |
| 6 | 4 | 3 | 6 | ← | 5 | 4 | 2 | 5 | 13396.5840 | -0.0134 |
| 6 | 4 | 3 | 5 | ← | 5 | 4 | 2 | 6 | 13397.1267 | 0.0019 |
| 6 | 4 | 2 | 5 | ← | 5 | 4 | 1 | 6 | 13398.2399 | 0.0074 |
| 6 | 3 | 4 | 7 | ← | 5 | 3 | 3 | 6 | 13410.5923 | -0.0074 |
| 6 | 2 | 4 | 5 | ← | 5 | 2 | 3 | 4 | 13742.3165 | -0.0221 |
| 4 | 2 | 3 | 3 | ← | 3 | 1 | 2 | 2 | 14151.6452 | -0.0122 |
| 4 | 2 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 14151.8550 | -0.0126 |
| 4 | 2 | 2 | 3 | ← | 3 | 1 | 2 | 2 | 14381.9274 | 0.0066 |
| 4 | 2 | 2 | 5 | ← | 3 | 1 | 2 | 4 | 14382.1246 | 0.0080 |
| 4 | 2 | 2 | 4 | ← | 3 | 1 | 2 | 3 | 14382.5442 | 0.0085 |
| 4 | 2 | 2 | 3 | ← | 3 | 1 | 2 | 3 | 14383.2022 | 0.0018 |
| 3 | 2 | 1 | 2 | ← | 2 | 0 | 2 | 1 | 14587.2827 | -0.0085 |
| 3 | 2 | 1 | 4 | ← | 2 | 0 | 2 | 3 | 14587.8985 | 0.0020 |
| 7 | 1 | 7 | 7 | ← | 6 | 1 | 6 | 6 | 14694.0782 | 0.0118 |
| 7 | 1 | 7 | 6 | ← | 6 | 1 | 6 | 5 | 14694.0782 | 0.0101 |
| 7 | 1 | 7 | 8 | ← | 6 | 1 | 6 | 7 | 14694.0782 | -0.0117 |
| 7 | 0 | 7 | 8 | ← | 6 | 0 | 6 | 7 | 14888.8147 | 0.0132 |
| 7 | 0 | 7 | 7 | ← | 6 | 0 | 6 | 6 | 14888.8147 | 0.0035 |
| 4 | 2 | 3 | 5 | ← | 3 | 1 | 3 | 4 | 15368.3934 | -0.0024 |
| 4 | 2 | 3 | 4 | ← | 3 | 1 | 3 | 3 | 15368.7093 | -0.0027 |
| 3 | 3 | 0 | 3 | ← | 2 | 2 | 0 | 2 | 16444.5314 | -0.0212 |
| 8 | 0 | 8 | 7 | ← | 7 | 0 | 7 | 6 | 16891.1955 | -0.0199 |
| 8 | 2 | 7 | 8 | ← | 7 | 2 | 6 | 7 | 17602.7435 | -0.0108 |
| 5 | 2 | 4 | 5 | ← | 4 | 1 | 4 | 4 | 17992.6563 | -0.0122 |
| 8 | 3 | 5 | 9 | ← | 7 | 3 | 4 | 8 | 18072.8910 | -0.0263 |
| 8 | 3 | 5 | 7 | ← | 7 | 3 | 4 | 6 | 18072.8910 | -0.0330 |
| 8 | 1 | 7 | 7 | ← | 7 | 1 | 6 | 6 | 18195.1661 | 0.0208 |
| 8 | 1 | 7 | 8 | ← | 7 | 1 | 6 | 7 | 18195.1661 | 0.0004 |
| 8 | 1 | 7 | 9 | ← | 7 | 1 | 6 | 8 | 18195.1661 | -0.0008 |
| 8 | 2 | 6 | 8 | ← | 7 | 2 | 5 | 8 | 18492.0596 | 0.0179 |
| 8 | 2 | 6 | 7 | ← | 7 | 2 | 5 | 6 | 18493.1899 | 0.0178 |
| 8 | 2 | 6 | 9 | ← | 7 | 2 | 5 | 8 | 18493.1899 | 0.0070 |
| 9 | 0 | 9 | 9 | ← | 8 | 1 | 8 | 8 | 18620.1856 | 0.0194 |
| 9 | 0 | 9 | 8 | ← | 8 | 1 | 8 | 7 | 18620.1856 | 0.0025 |
| 9 | 0 | 9 | 10 | ← | 8 | 1 | 8 | 9 | 18620.1856 | -0.0093 |
| 4 | 3 | 2 | 5 | ← | 3 | 2 | 1 | 4 | 18634.3306 | -0.0209 |
| 4 | 3 | 2 | 4 | ← | 3 | 2 | 1 | 4 | 18634.7390 | -0.0196 |
| 4 | 3 | 1 | 5 | ← | 3 | 2 | 1 | 4 | 18639.6889 | -0.0162 |
| 4 | 3 | 1 | 4 | ← | 3 | 2 | 1 | 4 | 18640.0979 | -0.0120 |
| 4 | 3 | 2 | 5 | ← | 3 | 2 | 2 | 4 | 18712.5002 | -0.0039 |
| 4 | 3 | 1 | 5 | ← | 3 | 2 | 2 | 4 | 18717.8450 | -0.0127 |
| 9 | 1 | 9 | 8 | ← | 8 | 1 | 8 | 7 | 18792.7226 | 0.0146 |
| 9 | 1 | 9 | 9 | ← | 8 | 1 | 8 | 8 | 18792.7226 | 0.0104 |
| 9 | 1 | 9 | 10 | ← | 8 | 1 | 8 | 9 | 18792.7226 | 0.0006 |
| 9 | 0 | 9 | 9 | ← | 8 | 0 | 8 | 9 | 18890.6529 | 0.0028 |
| 9 | 0 | 9 | 8 | ← | 8 | 0 | 8 | 7 | 18891.7522 | 0.0233 |
| 9 | 0 | 9 | 10 | ← | 8 | 0 | 8 | 9 | 18891.7522 | 0.0073 |
| 9 | 0 | 9 | 9 | ← | 8 | 0 | 8 | 8 | 18891.7522 | 0.0036 |
| 9 | 1 | 9 | 10 | ← | 8 | 0 | 8 | 9 | 19064.2852 | 0.0133 |
| 9 | 1 | 9 | 9 | ← | 8 | 0 | 8 | 8 | 19064.2852 | -0.0093 |
| 7 | 3 | 4 | 6 | ← | 7 | 1 | 7 | 6 | 19248.9858 | -0.0033 |
| 9 | 2 | 8 | 9 | ← | 8 | 2 | 7 | 8 | 19741.0817 | 0.0283 |
| 9 | 2 | 8 | 8 | ← | 8 | 2 | 7 | 7 | 19741.0817 | 0.0006 |
| 9 | 2 | 8 | 10 | ← | 8 | 2 | 7 | 9 | 19741.0817 | -0.0093 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | 5 | 4 | 10 | ← | 8 | 5 | 3 | 9 | 20119.9543 | 0.0200 |
| 9 | 3 | 7 | 8 | ← | 8 | 3 | 6 | 7 | 20132.9862 | 0.0319 |
| 9 | 4 | 6 | 10 | ← | 8 | 4 | 5 | 9 | 20157.1737 | -0.0238 |
| 9 | 4 | 5 | 10 | ← | 8 | 4 | 4 | 9 | 20180.6532 | -0.0244 |
| 10 | 4 | 7 | 9 | ← | 10 | 2 | 8 | 9 | 20205.5677 | 0.0109 |
| 9 | 1 | 8 | 8 | ← | 8 | 1 | 7 | 7 | 20315.6181 | 0.0166 |
| 9 | 1 | 8 | 10 | ← | 8 | 1 | 7 | 9 | 20315.6181 | -0.0012 |
| 9 | 1 | 8 | 9 | ← | 8 | 1 | 7 | 8 | 20315.6181 | -0.0088 |
| 9 | 1 | 8 | 8 | ← | 8 | 1 | 7 | 8 | 20316.9540 | 0.0040 |
| 9 | 3 | 6 | 9 | ← | 8 | 3 | 5 | 9 | 20434.1099 | 0.0302 |
| 9 | 3 | 6 | 10 | ← | 8 | 3 | 5 | 9 | 20435.0209 | -0.0046 |
| 9 | 3 | 6 | 8 | ← | 8 | 3 | 5 | 7 | 20435.0209 | -0.0056 |
| 10 | 0 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 20722.9321 | 0.0138 |
| 10 | 0 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 20722.9321 | 0.0066 |
| 10 | 0 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 20722.9321 | -0.0037 |
| 5 | 3 | 3 | 6 | ← | 4 | 2 | 2 | 5 | 20765.0309 | -0.0139 |
| 5 | 3 | 2 | 6 | ← | 4 | 2 | 2 | 5 | 20786.2919 | -0.0233 |
| 7 | 1 | 6 | 8 | ← | 6 | 0 | 6 | 7 | 20829.2860 | 0.0247 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 20830.0054 | 0.0126 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 20830.0054 | 0.0078 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 20830.0054 | 0.0011 |
| 9 | 2 | 7 | 9 | ← | 8 | 2 | 6 | 8 | 20841.2750 | 0.0267 |
| 9 | 2 | 7 | 8 | ← | 8 | 2 | 6 | 7 | 20841.2750 | -0.0073 |
| 9 | 2 | 7 | 10 | ← | 8 | 2 | 6 | 9 | 20841.2750 | -0.0184 |
| 9 | 2 | 7 | 9 | ← | 8 | 2 | 6 | 8 | 20841.2750 | 0.0267 |
| 9 | 2 | 7 | 8 | ← | 8 | 2 | 6 | 7 | 20841.2750 | -0.0073 |
| 9 | 2 | 7 | 10 | ← | 8 | 2 | 6 | 9 | 20841.2750 | -0.0184 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 20895.4675 | 0.0170 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 20895.4675 | 0.0045 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 20895.4675 | 0.0031 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 20895.4675 | 0.0170 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 20895.4675 | 0.0045 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 20895.4675 | 0.0031 |
| 5 | 3 | 3 | 6 | ← | 4 | 2 | 3 | 5 | 20995.2990 | 0.0051 |
| 5 | 3 | 3 | 4 | ← | 4 | 2 | 3 | 5 | 20995.2990 | -0.0223 |
| 7 | 2 | 5 | 6 | ← | 6 | 1 | 5 | 5 | 20998.8243 | 0.0274 |
| 7 | 2 | 5 | 8 | ← | 6 | 1 | 5 | 7 | 20998.8243 | -0.0175 |
| 10 | 1 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 21002.5142 | -0.0034 |
| 10 | 1 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 21002.5142 | -0.0170 |
| 10 | 1 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 21002.5142 | -0.0293 |
| 5 | 3 | 2 | 6 | ← | 4 | 2 | 3 | 5 | 21016.5845 | 0.0202 |
| 6 | 2 | 4 | 7 | ← | 5 | 1 | 5 | 6 | 21703.4381 | 0.0078 |
| 6 | 2 | 4 | 6 | ← | 5 | 1 | 5 | 5 | 21703.4381 | -0.0165 |
| 10 | 2 | 9 | 10 | ← | 9 | 2 | 8 | 9 | 21860.7977 | 0.0133 |
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 8 | 21860.7977 | -0.0025 |
| 10 | 2 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 21860.7977 | -0.0117 |
| 10 | 2 | 9 | 10 | ← | 9 | 2 | 8 | 9 | 21860.7977 | 0.0133 |
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 8 | 21860.7977 | -0.0025 |
| 10 | 2 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 21860.7977 | -0.0117 |
| 10 | 8 | 2 | 9 | ← | 9 | 8 | 1 | 8 | 22307.8679 | -0.0025 |
| 10 | 8 | 3 | 9 | ← | 9 | 8 | 2 | 8 | 22307.8679 | -0.0025 |
| 10 | 7 | 4 | 10 | ← | 9 | 7 | 3 | 9 | 22320.4301 | 0.0041 |
| 10 | 7 | 3 | 10 | ← | 9 | 7 | 2 | 9 | 22320.4301 | 0.0034 |
| 10 | 7 | 4 | 11 | ← | 9 | 7 | 3 | 10 | 22320.8179 | 0.0211 |
| 10 | 7 | 3 | 11 | ← | 9 | 7 | 2 | 10 | 22320.8179 | 0.0204 |
| 10 | 7 | 4 | 9 | ← | 9 | 7 | 3 | 8 | 22320.8179 | -0.0249 |
| 10 | 7 | 3 | 9 | ← | 9 | 7 | 2 | 8 | 22320.8179 | -0.0256 |
| 10 | 6 | 5 | 10 | ← | 9 | 6 | 4 | 9 | 22340.8951 | -0.0007 |
| 10 | 6 | 4 | 10 | ← | 9 | 6 | 3 | 10 | 22341.2092 | 0.0235 |
| 10 | 6 | 5 | 9 | ← | 9 | 6 | 4 | 8 | 22341.2092 | 0.0081 |
| 10 | 6 | 4 | 11 | ← | 9 | 6 | 3 | 10 | 22341.2092 | -0.0137 |
| 10 | 6 | 4 | 10 | ← | 9 | 6 | 3 | 10 | 22341.2092 | 0.0235 |
| 10 | 6 | 5 | 9 | ← | 9 | 6 | 4 | 8 | 22341.2092 | 0.0081 |
| 10 | 6 | 4 | 11 | ← | 9 | 6 | 3 | 10 | 22341.2092 | -0.0137 |
| 10 | 6 | 4 | 9 | ← | 9 | 6 | 3 | 10 | 22341.2092 | -0.0176 |
| 10 | 3 | 8 | 9 | ← | 9 | 3 | 7 | 8 | 22358.3439 | 0.0038 |
| 10 | 3 | 8 | 11 | ← | 9 | 3 | 7 | 10 | 22358.3439 | 0.0007 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | 5 | 5 | 11 | ← | 9 | 5 | 4 | 10 | 22377.2015 | -0.0191 |
| 10 | 1 | 9 | 9 | ← | 9 | 1 | 8 | 8 | 22383.4194 | 0.0113 |
| 10 | 1 | 9 | 11 | ← | 9 | 1 | 8 | 10 | 22383.4194 | -0.0033 |
| 10 | 1 | 9 | 10 | ← | 9 | 1 | 8 | 9 | 22383.4194 | -0.0164 |
| 10 | 4 | 7 | 11 | ← | 9 | 4 | 6 | 10 | 22420.3407 | 0.0007 |
| 10 | 4 | 7 | 9 | ← | 9 | 4 | 6 | 8 | 22420.3407 | -0.0051 |
| 10 | 4 | 6 | 11 | ← | 9 | 4 | 5 | 10 | 22469.9477 | -0.0006 |
| 10 | 4 | 6 | 9 | ← | 9 | 4 | 5 | 8 | 22469.9477 | -0.0069 |
| 10 | 3 | 7 | 9 | ← | 9 | 3 | 6 | 8 | 22831.3376 | 0.0271 |
| 10 | 3 | 7 | 11 | ← | 9 | 3 | 6 | 10 | 22831.3376 | 0.0254 |
| 11 | 1 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 22861.8030 | 0.0065 |
| 11 | 1 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 22861.8030 | 0.0018 |
| 11 | 1 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 22861.8030 | -0.0029 |
| 6 | 3 | 3 | 7 | ← | 5 | 2 | 3 | 6 | 22864.1118 | 0.0063 |
| 11 | 0 | 11 | 10 | ← | 10 | 0 | 10 | 9 | 22903.6443 | 0.0074 |
| 11 | 0 | 11 | 11 | ← | 10 | 0 | 10 | 10 | 22903.6443 | -0.0026 |
| 11 | 0 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 22903.6443 | -0.0026 |
| 11 | 1 | 11 | 10 | ← | 10 | 0 | 10 | 9 | 22968.8394 | -0.0242 |
| 10 | 2 | 8 | 10 | ← | 9 | 2 | 7 | 9 | 23154.9476 | -0.0014 |
| 10 | 2 | 8 | 9 | ← | 9 | 2 | 7 | 8 | 23154.9476 | -0.0183 |
| 10 | 2 | 8 | 11 | ← | 9 | 2 | 7 | 10 | 23154.9476 | -0.0289 |
| 6 | 3 | 4 | 5 | ← | 5 | 2 | 4 | 4 | 23320.9465 | 0.0294 |
| 6 | 3 | 4 | 6 | ← | 5 | 2 | 4 | 5 | 23321.2178 | -0.0329 |
| 6 | 3 | 3 | 5 | ← | 5 | 2 | 4 | 4 | 23383.9963 | 0.0167 |
| 8 | 2 | 6 | 7 | ← | 7 | 1 | 6 | 6 | 23469.4841 | 0.0189 |
| 8 | 2 | 6 | 9 | ← | 7 | 1 | 6 | 8 | 23469.4841 | -0.0099 |
| 7 | 2 | 6 | 6 | ← | 6 | 1 | 6 | 5 | 23531.8329 | -0.0127 |
| 11 | 2 | 10 | 11 | ← | 10 | 2 | 9 | 10 | 23962.3003 | -0.0009 |
| 11 | 2 | 10 | 10 | ← | 10 | 2 | 9 | 9 | 23962.3003 | -0.0094 |
| 11 | 2 | 10 | 12 | ← | 10 | 2 | 9 | 11 | 23962.3003 | -0.0176 |
| 10 | 2 | 9 | 9 | ← | 9 | 1 | 8 | 8 | 24005.9337 | -0.0038 |
| 10 | 2 | 9 | 11 | ← | 9 | 1 | 8 | 10 | 24005.9337 | -0.0298 |
| 11 | 1 | 10 | 10 | ← | 10 | 1 | 9 | 9 | 24406.7527 | 0.0006 |
| 11 | 1 | 10 | 12 | ← | 10 | 1 | 9 | 11 | 24406.7527 | -0.0115 |
| 11 | 1 | 10 | 11 | ← | 10 | 1 | 9 | 10 | 24406.7527 | -0.0264 |
| 11 | 7 | 5 | 10 | ← | 10 | 7 | 4 | 11 | 24565.4497 | 0.0114 |
| 11 | 7 | 4 | 10 | ← | 10 | 7 | 3 | 11 | 24565.4497 | 0.0084 |
| 11 | 7 | 5 | 12 | ← | 10 | 7 | 4 | 11 | 24565.4497 | -0.0003 |
| 11 | 7 | 4 | 12 | ← | 10 | 7 | 3 | 11 | 24565.4497 | -0.0033 |
| 11 | 7 | 5 | 10 | ← | 10 | 7 | 4 | 9 | 24565.4497 | -0.0297 |
| 11 | 7 | 4 | 10 | ← | 10 | 7 | 3 | 9 | 24565.4497 | -0.0327 |
| 11 | 3 | 9 | 11 | ← | 10 | 3 | 8 | 10 | 24569.8995 | 0.0249 |
| 11 | 3 | 9 | 10 | ← | 10 | 3 | 8 | 9 | 24569.8995 | -0.0212 |
| 11 | 6 | 6 | 10 | ← | 10 | 6 | 5 | 10 | 24592.7233 | 0.0192 |
| 11 | 5 | 7 | 11 | ← | 10 | 5 | 6 | 10 | 24636.7690 | -0.0072 |
| 11 | 4 | 8 | 12 | ← | 10 | 4 | 7 | 11 | 24685.8030 | 0.0208 |
| 11 | 4 | 8 | 10 | ← | 10 | 4 | 7 | 9 | 24685.8030 | 0.0187 |
| 11 | 4 | 7 | 12 | ← | 10 | 4 | 6 | 11 | 24781.5704 | 0.0219 |
| 11 | 4 | 7 | 10 | ← | 10 | 4 | 6 | 9 | 24781.5704 | 0.0199 |
| 12 | 0 | 12 | 13 | ← | 11 | 1 | 11 | 12 | 24850.5990 | 0.0329 |
| 7 | 3 | 4 | 7 | ← | 6 | 2 | 4 | 6 | 24868.8862 | -0.0307 |
| 12 | 1 | 12 | 11 | ← | 11 | 1 | 11 | 10 | 24889.7078 | -0.0015 |
| 12 | 1 | 12 | 12 | ← | 11 | 1 | 11 | 11 | 24889.7078 | -0.0060 |
| 12 | 1 | 12 | 13 | ← | 11 | 1 | 11 | 12 | 24889.7078 | -0.0096 |
| 12 | 0 | 12 | 11 | ← | 11 | 0 | 11 | 10 | 24915.7840 | -0.0011 |
| 12 | 0 | 12 | 12 | ← | 11 | 0 | 11 | 11 | 24915.7840 | -0.0085 |
| 12 | 0 | 12 | 13 | ← | 11 | 0 | 11 | 12 | 24915.7840 | -0.0094 |
| 12 | 1 | 11 | 11 | ← | 11 | 2 | 10 | 10 | 25222.7026 | 0.0195 |
| 12 | 1 | 11 | 13 | ← | 11 | 2 | 10 | 12 | 25222.7026 | 0.0167 |
| 11 | 3 | 8 | 10 | ← | 10 | 3 | 7 | 9 | 25250.9277 | -0.0099 |
| 11 | 3 | 8 | 12 | ← | 10 | 3 | 7 | 11 | 25250.9277 | -0.0131 |
| 11 | 2 | 9 | 11 | ← | 10 | 2 | 8 | 10 | 25425.8187 | -0.0190 |
| 11 | 2 | 9 | 10 | ← | 10 | 2 | 8 | 9 | 25425.8187 | -0.0235 |
| 7 | 3 | 5 | 8 | ← | 6 | 2 | 5 | 7 | 25703.0630 | 0.0021 |
| | | | | | | | | | RMS | 11.2 kHz |

Table S12 Linelist for Conformer IV of isoleucinol. OMC is the difference between the observed and calculated transition.

| J' | $K_{a'}$ | $K_{c'}$ | F' | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 1 | 1 | ← | 0 | 0 | 0 | 1 | 2055.2274 | -0.0047 |
| 1 | 0 | 1 | 2 | ← | 0 | 0 | 0 | 1 | 2056.3406 | 0.0028 |
| 1 | 0 | 1 | 0 | ← | 0 | 0 | 0 | 1 | 2057.9952 | -0.0013 |
| 2 | 1 | 1 | 1 | ← | 2 | 0 | 2 | 1 | 2376.5824 | -0.0015 |
| 2 | 1 | 1 | 3 | ← | 2 | 0 | 2 | 3 | 2376.9060 | 0.0090 |
| 2 | 1 | 1 | 2 | ← | 2 | 0 | 2 | 2 | 2377.4669 | 0.0060 |
| 3 | 1 | 2 | 2 | ← | 3 | 0 | 3 | 2 | 2557.2053 | 0.0057 |
| 3 | 1 | 2 | 4 | ← | 3 | 0 | 3 | 4 | 2557.3032 | 0.0075 |
| 3 | 1 | 2 | 3 | ← | 3 | 0 | 3 | 3 | 2557.5735 | 0.0032 |
| 4 | 1 | 3 | 5 | ← | 4 | 0 | 4 | 5 | 2811.8639 | 0.0006 |
| 4 | 1 | 3 | 4 | ← | 4 | 0 | 4 | 4 | 2812.0124 | -0.0023 |
| 2 | 1 | 2 | 2 | ← | 1 | 1 | 1 | 1 | 4000.4928 | -0.0026 |
| 2 | 1 | 2 | 2 | ← | 1 | 1 | 1 | 2 | 4001.0729 | 0.0004 |
| 2 | 1 | 2 | 1 | ← | 1 | 1 | 1 | 1 | 4001.3744 | -0.0024 |
| 2 | 1 | 2 | 3 | ← | 1 | 1 | 1 | 2 | 4001.6356 | -0.0030 |
| 2 | 1 | 2 | 1 | ← | 1 | 1 | 1 | 0 | 4002.8210 | 0.0015 |
| 3 | 0 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 4106.9473 | -0.0037 |
| 2 | 0 | 2 | 2 | ← | 1 | 0 | 1 | 2 | 4107.0235 | -0.0001 |
| 2 | 0 | 2 | 1 | ← | 1 | 0 | 1 | 0 | 4107.2062 | 0.0019 |
| 3 | 0 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 4107.6062 | -0.0009 |
| 2 | 0 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 4108.2034 | -0.0023 |
| 3 | 0 | 3 | 2 | ← | 2 | 1 | 2 | 2 | 4108.5968 | -0.0045 |
| 2 | 0 | 2 | 1 | ← | 1 | 0 | 1 | 1 | 4109.9638 | -0.0047 |
| 1 | 1 | 1 | 0 | ← | 0 | 0 | 0 | 1 | 4206.2549 | -0.0021 |
| 1 | 1 | 1 | 2 | ← | 0 | 0 | 0 | 1 | 4207.1216 | -0.0010 |
| 1 | 1 | 1 | 1 | ← | 0 | 0 | 0 | 1 | 4207.6993 | -0.0003 |
| 2 | 1 | 1 | 2 | ← | 1 | 1 | 0 | 1 | 4222.2814 | 0.0078 |
| 2 | 1 | 1 | 2 | ← | 1 | 1 | 0 | 2 | 4222.8013 | -0.0004 |
| 2 | 1 | 1 | 1 | ← | 1 | 1 | 0 | 1 | 4223.2429 | 0.0069 |
| 2 | 1 | 1 | 3 | ← | 1 | 1 | 0 | 2 | 4223.4214 | 0.0013 |
| 2 | 1 | 1 | 1 | ← | 1 | 1 | 0 | 0 | 4224.5569 | 0.0000 |
| 5 | 1 | 4 | 5 | ← | 4 | 2 | 3 | 4 | 4464.9855 | -0.0045 |
| 5 | 1 | 4 | 6 | ← | 4 | 2 | 3 | 5 | 4465.6620 | 0.0016 |
| 5 | 1 | 4 | 4 | ← | 4 | 2 | 3 | 3 | 4465.7709 | 0.0009 |
| 8 | 2 | 6 | 9 | ← | 8 | 1 | 7 | 9 | 5543.1637 | -0.0007 |
| 8 | 2 | 6 | 8 | ← | 8 | 1 | 7 | 8 | 5543.3110 | -0.0001 |
| 7 | 2 | 5 | 8 | ← | 7 | 1 | 6 | 8 | 5631.9121 | -0.0024 |
| 7 | 2 | 5 | 7 | ← | 7 | 1 | 6 | 7 | 5632.1119 | -0.0034 |
| 6 | 2 | 4 | 6 | ← | 6 | 1 | 5 | 6 | 5775.0480 | -0.0021 |
| 5 | 2 | 3 | 4 | ← | 5 | 1 | 4 | 4 | 5949.8444 | -0.0092 |
| 5 | 2 | 3 | 6 | ← | 5 | 1 | 4 | 6 | 5949.9279 | -0.0052 |
| 5 | 2 | 3 | 5 | ← | 5 | 1 | 4 | 5 | 5950.3180 | -0.0060 |
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 3 | 5998.7597 | -0.0022 |
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 5999.3262 | -0.0020 |
| 3 | 1 | 3 | 2 | ← | 2 | 1 | 2 | 1 | 5999.6528 | -0.0006 |
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 5999.6528 | -0.0027 |
| 3 | 1 | 3 | 2 | ← | 2 | 1 | 2 | 2 | 6000.5332 | -0.0016 |
| 4 | 2 | 2 | 3 | ← | 4 | 1 | 3 | 3 | 6135.1047 | -0.0002 |
| 4 | 2 | 2 | 5 | ← | 4 | 1 | 3 | 5 | 6135.2557 | 0.0015 |
| 4 | 2 | 2 | 4 | ← | 4 | 1 | 3 | 4 | 6135.8349 | 0.0007 |
| 3 | 0 | 3 | 3 | ← | 2 | 0 | 2 | 3 | 6150.6045 | 0.0018 |
| 2 | 1 | 2 | 1 | ← | 1 | 0 | 1 | 0 | 6151.0849 | 0.0049 |
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 1 | 6151.5947 | -0.0010 |
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 6151.8150 | -0.0098 |
| 2 | 1 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 6152.4238 | 0.0003 |
| 2 | 1 | 2 | 2 | ← | 1 | 0 | 1 | 1 | 6152.9612 | -0.0016 |
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 2 | 6153.4349 | -0.0002 |
| 2 | 1 | 2 | 1 | ← | 1 | 0 | 1 | 1 | 6153.8456 | 0.0012 |
| 3 | 2 | 2 | 3 | ← | 2 | 2 | 1 | 2 | 6167.5392 | 0.0034 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 2 | 6167.5392 | 0.0031 |
| 3 | 2 | 2 | 4 | ← | 2 | 2 | 1 | 3 | 6168.7224 | 0.0021 |
| 3 | 2 | 2 | 3 | ← | 2 | 2 | 1 | 3 | 6168.7224 | 0.0020 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 3 | 6168.7224 | 0.0017 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 1 | 6169.3802 | 0.0015 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 2 | 1 | 3 | ← | 2 | 2 | 0 | 2 | 6184.2098 | 0.0071 |
| 3 | 2 | 1 | 2 | ← | 2 | 2 | 0 | 2 | 6184.2098 | -0.0015 |
| 3 | 2 | 1 | 3 | ← | 2 | 2 | 0 | 3 | 6185.3969 | 0.0120 |
| 3 | 2 | 1 | 4 | ← | 2 | 2 | 0 | 3 | 6185.3969 | 0.0058 |
| 3 | 2 | 1 | 2 | ← | 2 | 2 | 0 | 3 | 6185.3969 | 0.0033 |
| 3 | 2 | 1 | 2 | ← | 2 | 2 | 0 | 1 | 6186.0595 | 0.0093 |
| 4 | 0 | 4 | 4 | ← | 3 | 1 | 3 | 4 | 6289.9035 | -0.0030 |
| 4 | 0 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 6290.7946 | -0.0054 |
| 4 | 0 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 6291.1490 | -0.0026 |
| 4 | 0 | 4 | 3 | ← | 3 | 1 | 3 | 2 | 6291.1490 | -0.0098 |
| 4 | 0 | 4 | 3 | ← | 3 | 1 | 3 | 3 | 6292.3578 | -0.0077 |
| 3 | 2 | 1 | 3 | ← | 3 | 1 | 2 | 2 | 6309.7851 | 0.0049 |
| 3 | 2 | 1 | 2 | ← | 3 | 1 | 2 | 2 | 6309.7851 | -0.0038 |
| 3 | 2 | 1 | 3 | ← | 3 | 1 | 2 | 4 | 6310.1158 | 0.0037 |
| 3 | 2 | 1 | 4 | ← | 3 | 1 | 2 | 4 | 6310.1158 | -0.0024 |
| 3 | 2 | 1 | 3 | ← | 3 | 1 | 2 | 3 | 6311.0598 | 0.0001 |
| 3 | 2 | 1 | 4 | ← | 3 | 1 | 2 | 3 | 6311.0598 | -0.0060 |
| 3 | 2 | 1 | 2 | ← | 3 | 1 | 2 | 3 | 6311.0598 | -0.0086 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 3 | 6331.2692 | -0.0067 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 6331.8882 | -0.0060 |
| 3 | 1 | 2 | 2 | ← | 2 | 1 | 1 | 1 | 6332.2201 | 0.0087 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6332.2201 | -0.0033 |
| 3 | 1 | 2 | 2 | ← | 2 | 1 | 1 | 2 | 6333.1706 | -0.0032 |
| 2 | 2 | 0 | 1 | ← | 2 | 1 | 1 | 1 | 6455.9516 | 0.0016 |
| 2 | 2 | 0 | 3 | ← | 2 | 1 | 1 | 3 | 6456.9546 | 0.0038 |
| 2 | 2 | 0 | 2 | ← | 2 | 1 | 1 | 2 | 6458.7600 | 0.0086 |
| 2 | 2 | 1 | 1 | ← | 2 | 1 | 2 | 1 | 6784.4712 | -0.0077 |
| 2 | 2 | 1 | 3 | ← | 2 | 1 | 2 | 3 | 6785.4595 | 0.0072 |
| 2 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 1 | 6786.3156 | -0.0059 |
| 2 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 2 | 6787.1911 | -0.0118 |
| 6 | 1 | 5 | 6 | ← | 5 | 2 | 4 | 5 | 6826.9747 | 0.0078 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 2 | 6954.1942 | -0.0096 |
| 3 | 2 | 2 | 2 | ← | 3 | 1 | 3 | 2 | 6954.1942 | -0.0099 |
| 3 | 2 | 2 | 4 | ← | 3 | 1 | 3 | 4 | 6954.5258 | 0.0088 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 4 | 6954.5258 | 0.0087 |
| 3 | 2 | 2 | 4 | ← | 3 | 1 | 3 | 3 | 6955.4164 | 0.0059 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 3 | 6955.4164 | 0.0058 |
| 3 | 2 | 2 | 2 | ← | 3 | 1 | 3 | 3 | 6955.4164 | 0.0055 |
| 4 | 2 | 3 | 3 | ← | 4 | 1 | 4 | 3 | 7181.0543 | -0.0009 |
| 4 | 2 | 3 | 5 | ← | 4 | 1 | 4 | 5 | 7181.2011 | 0.0080 |
| 4 | 2 | 3 | 4 | ← | 4 | 1 | 4 | 4 | 7181.7308 | 0.0011 |
| 4 | 2 | 3 | 5 | ← | 4 | 1 | 4 | 4 | 7182.2302 | -0.0013 |
| 5 | 2 | 4 | 6 | ← | 5 | 1 | 5 | 6 | 7466.4321 | -0.0154 |
| 5 | 2 | 4 | 5 | ← | 5 | 1 | 5 | 5 | 7466.8001 | -0.0003 |
| 4 | 1 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 7994.8240 | 0.0151 |
| 3 | 1 | 3 | 3 | ← | 2 | 0 | 2 | 3 | 8042.9820 | 0.0022 |
| 3 | 1 | 3 | 2 | ← | 2 | 0 | 2 | 1 | 8043.5295 | 0.0003 |
| 3 | 1 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 8043.8713 | -0.0019 |
| 3 | 1 | 3 | 3 | ← | 2 | 0 | 2 | 2 | 8044.1620 | 0.0001 |
| 3 | 1 | 3 | 2 | ← | 2 | 0 | 2 | 2 | 8045.3649 | -0.0037 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 4 | 8181.9518 | -0.0032 |
| 4 | 0 | 4 | 3 | ← | 3 | 0 | 3 | 2 | 8183.0767 | -0.0155 |
| 4 | 0 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 8183.2147 | 0.0146 |
| 4 | 0 | 4 | 3 | ← | 3 | 0 | 3 | 3 | 8184.7388 | -0.0038 |
| 4 | 2 | 3 | 4 | ← | 3 | 2 | 2 | 3 | 8220.9800 | -0.0030 |
| 4 | 2 | 3 | 4 | ← | 3 | 2 | 2 | 4 | 8220.9800 | -0.0031 |
| 4 | 2 | 3 | 5 | ← | 3 | 2 | 2 | 4 | 8221.4950 | 0.0099 |
| 4 | 3 | 1 | 4 | ← | 3 | 3 | 0 | 3 | 8232.4404 | 0.0073 |
| 4 | 2 | 2 | 4 | ← | 3 | 2 | 1 | 4 | 8262.3909 | 0.0008 |
| 4 | 2 | 2 | 4 | ← | 3 | 2 | 1 | 3 | 8262.3909 | -0.0053 |
| 4 | 2 | 2 | 5 | ← | 3 | 2 | 1 | 4 | 8262.9052 | 0.0018 |
| 4 | 1 | 3 | 4 | ← | 3 | 1 | 2 | 4 | 8436.6735 | -0.0007 |
| 4 | 1 | 3 | 4 | ← | 3 | 1 | 2 | 3 | 8437.6088 | -0.0129 |
| 4 | 1 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 8437.7579 | -0.0096 |
| 4 | 1 | 3 | 3 | ← | 3 | 1 | 2 | 3 | 8438.9788 | -0.0178 |
| 5 | 0 | 5 | 5 | ← | 4 | 1 | 4 | 4 | 8495.0625 | 0.0019 |
| 5 | 0 | 5 | 4 | ← | 4 | 1 | 4 | 3 | 8495.2840 | 0.0145 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | 0 | 5 | 6 | ← | 4 | 1 | 4 | 5 | 8495.2840 | 0.0037 |
| 3 | 1 | 2 | 4 | ← | 2 | 0 | 2 | 3 | 8709.1216 | 0.0011 |
| 3 | 1 | 2 | 3 | ← | 2 | 0 | 2 | 2 | 8709.3577 | 0.0026 |
| 4 | 1 | 4 | 4 | ← | 3 | 0 | 3 | 4 | 9885.8371 | 0.0181 |
| 4 | 1 | 4 | 3 | ← | 3 | 0 | 3 | 2 | 9886.7048 | 0.0083 |
| 4 | 1 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 9886.8486 | -0.0087 |
| 4 | 1 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 9887.0348 | -0.0064 |
| 4 | 1 | 4 | 3 | ← | 3 | 0 | 3 | 3 | 9888.3582 | 0.0113 |
| 5 | 1 | 5 | 6 | ← | 4 | 1 | 4 | 5 | 9986.2936 | 0.0121 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 5 | 10197.6579 | -0.0215 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 10198.9134 | -0.0110 |
| 5 | 0 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 10198.9134 | -0.0241 |
| 5 | 0 | 5 | 4 | ← | 4 | 0 | 4 | 4 | 10200.4505 | 0.0114 |
| 5 | 2 | 4 | 5 | ← | 4 | 2 | 3 | 5 | 10270.7771 | 0.0051 |
| 5 | 2 | 4 | 5 | ← | 4 | 2 | 3 | 4 | 10271.2703 | -0.0035 |
| 5 | 2 | 4 | 6 | ← | 4 | 2 | 3 | 5 | 10271.5282 | -0.0075 |
| 5 | 2 | 4 | 4 | ← | 4 | 2 | 3 | 4 | 10272.1825 | -0.0110 |
| 5 | 4 | 2 | 6 | ← | 4 | 4 | 1 | 5 | 10290.3038 | 0.0111 |
| 5 | 4 | 1 | 6 | ← | 4 | 4 | 0 | 5 | 10290.3038 | -0.0042 |
| 5 | 3 | 3 | 5 | ← | 4 | 3 | 2 | 4 | 10293.6735 | -0.0068 |
| 5 | 3 | 3 | 6 | ← | 4 | 3 | 2 | 5 | 10294.2552 | 0.0064 |
| 5 | 3 | 2 | 5 | ← | 4 | 3 | 1 | 4 | 10295.7300 | -0.0109 |
| 5 | 3 | 2 | 6 | ← | 4 | 3 | 1 | 5 | 10296.3080 | -0.0017 |
| 5 | 2 | 3 | 5 | ← | 4 | 2 | 2 | 4 | 10353.0624 | 0.0038 |
| 5 | 2 | 3 | 6 | ← | 4 | 2 | 2 | 5 | 10353.3235 | -0.0032 |
| 5 | 1 | 4 | 5 | ← | 4 | 1 | 3 | 5 | 10537.4612 | -0.0140 |
| 5 | 1 | 4 | 6 | ← | 4 | 1 | 3 | 5 | 10538.6352 | -0.0124 |
| 5 | 1 | 4 | 4 | ← | 4 | 1 | 3 | 4 | 10539.9816 | 0.0015 |
| 2 | 2 | 1 | 1 | ← | 1 | 1 | 0 | 1 | 10675.0171 | 0.0103 |
| 2 | 2 | 1 | 3 | ← | 1 | 1 | 0 | 2 | 10676.1913 | -0.0018 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 0 | 1 | 10676.8425 | -0.0069 |
| 2 | 2 | 0 | 3 | ← | 1 | 1 | 0 | 2 | 10680.3599 | -0.0111 |
| 6 | 0 | 6 | 7 | ← | 5 | 1 | 5 | 6 | 10705.7772 | -0.0146 |
| 6 | 0 | 6 | 5 | ← | 5 | 1 | 5 | 4 | 10705.7772 | -0.0007 |
| 2 | 2 | 0 | 1 | ← | 1 | 1 | 1 | 1 | 10790.0351 | 0.0001 |
| 2 | 2 | 0 | 1 | ← | 1 | 1 | 1 | 2 | 10790.5950 | -0.0169 |
| 2 | 2 | 0 | 3 | ← | 1 | 1 | 1 | 2 | 10791.2717 | 0.0031 |
| 2 | 2 | 0 | 1 | ← | 1 | 1 | 1 | 0 | 10791.4755 | -0.0020 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 1 | 1 | 10791.8795 | 0.0057 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 1 | 2 | 10792.4571 | 0.0063 |
| 6 | 3 | 3 | 7 | ← | 6 | 2 | 4 | 7 | 10832.0563 | -0.0285 |
| 6 | 3 | 3 | 6 | ← | 6 | 2 | 4 | 6 | 10832.5559 | -0.0064 |
| 5 | 3 | 2 | 6 | ← | 5 | 2 | 3 | 6 | 10927.4683 | -0.0032 |
| 5 | 3 | 2 | 5 | ← | 5 | 2 | 3 | 5 | 10928.0988 | -0.0232 |
| 4 | 3 | 2 | 4 | ← | 4 | 2 | 2 | 5 | 10984.2518 | 0.0137 |
| 4 | 3 | 1 | 3 | ← | 4 | 2 | 2 | 3 | 10984.2518 | 0.0078 |
| 4 | 3 | 1 | 5 | ← | 4 | 2 | 2 | 5 | 10984.4843 | -0.0043 |
| 4 | 3 | 1 | 4 | ← | 4 | 2 | 2 | 4 | 10985.4273 | -0.0123 |
| 5 | 3 | 3 | 6 | ← | 5 | 2 | 4 | 6 | 11068.7601 | -0.0198 |
| 5 | 3 | 3 | 5 | ← | 5 | 2 | 4 | 5 | 11069.4067 | -0.0067 |
| 8 | 1 | 7 | 9 | ← | 7 | 2 | 6 | 8 | 11664.9980 | -0.0175 |
| 5 | 1 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 11690.0720 | 0.0050 |
| 6 | 0 | 6 | 6 | ← | 5 | 0 | 5 | 5 | 12196.7953 | 0.0095 |
| 6 | 0 | 6 | 7 | ← | 5 | 0 | 5 | 6 | 12196.7953 | 0.0023 |
| 6 | 0 | 6 | 5 | ← | 5 | 0 | 5 | 5 | 12198.2529 | -0.0120 |
| 6 | 2 | 5 | 6 | ← | 5 | 2 | 4 | 5 | 12317.9910 | 0.0053 |
| 6 | 2 | 5 | 5 | ← | 5 | 2 | 4 | 4 | 12318.1405 | 0.0007 |
| 6 | 2 | 5 | 7 | ← | 5 | 2 | 4 | 6 | 12318.1405 | 0.0002 |
| 6 | 2 | 4 | 5 | ← | 5 | 2 | 3 | 4 | 12458.1461 | 0.0075 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 1 | 12621.1425 | -0.0069 |
| 3 | 2 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 12621.4866 | -0.0066 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 1 | 3 | 12621.4866 | -0.0067 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 3 | 12621.4866 | -0.0069 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 12622.1086 | -0.0030 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 2 | 12622.1086 | -0.0033 |
| 7 | 0 | 7 | 6 | ← | 6 | 1 | 6 | 5 | 12908.5903 | -0.0058 |
| 7 | 0 | 7 | 8 | ← | 6 | 1 | 6 | 7 | 12908.5903 | -0.0194 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 1 | 12974.7002 | -0.0081 |
| 3 | 2 | 1 | 3 | ← | 2 | 1 | 2 | 3 | 12975.0208 | 0.0059 |
| 3 | 2 | 1 | 4 | ← | 2 | 1 | 2 | 3 | 12975.0208 | -0.0002 |
| 3 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 3 | 12975.0208 | -0.0028 |
| 3 | 2 | 1 | 3 | ← | 2 | 1 | 2 | 2 | 12975.5766 | -0.0044 |
| 3 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 2 | 12975.5766 | -0.0132 |
| 7 | 0 | 7 | 6 | ← | 6 | 0 | 6 | 5 | 14176.2782 | 0.0164 |
| 7 | 0 | 7 | 7 | ← | 6 | 0 | 6 | 6 | 14176.2782 | -0.0106 |
| 7 | 0 | 7 | 8 | ← | 6 | 0 | 6 | 7 | 14176.2782 | -0.0142 |
| 7 | 3 | 4 | 8 | ← | 6 | 3 | 3 | 7 | 14434.0935 | -0.0014 |
| 7 | 3 | 4 | 6 | ← | 6 | 3 | 3 | 5 | 14434.0935 | -0.0208 |
| 4 | 2 | 3 | 4 | ← | 3 | 1 | 2 | 4 | 14510.2765 | 0.0236 |
| 4 | 2 | 3 | 3 | ← | 3 | 1 | 2 | 2 | 14510.5278 | -0.0244 |
| 4 | 2 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 14510.7340 | -0.0208 |
| 4 | 2 | 3 | 4 | ← | 3 | 1 | 2 | 3 | 14511.1845 | -0.0159 |
| 4 | 2 | 2 | 5 | ← | 3 | 1 | 2 | 4 | 14573.0330 | 0.0113 |
| 7 | 2 | 5 | 6 | ← | 6 | 2 | 4 | 5 | 14577.0272 | -0.0225 |
| 7 | 1 | 6 | 8 | ← | 6 | 1 | 5 | 7 | 14719.9137 | -0.0029 |
| 4 | 2 | 3 | 5 | ← | 3 | 1 | 3 | 4 | 15176.0122 | 0.0101 |
| 4 | 2 | 2 | 5 | ← | 3 | 1 | 3 | 4 | 15238.2637 | -0.0051 |
| 4 | 2 | 2 | 4 | ← | 3 | 1 | 3 | 3 | 15238.6436 | -0.0054 |
| 3 | 3 | 1 | 2 | ← | 2 | 2 | 1 | 1 | 17203.4684 | 0.0153 |
| 9 | 0 | 9 | 9 | ← | 8 | 1 | 8 | 8 | 17246.4279 | 0.0064 |
| 5 | 2 | 3 | 6 | ← | 4 | 1 | 4 | 5 | 17596.7607 | -0.0260 |
| 5 | 2 | 3 | 5 | ← | 4 | 1 | 4 | 4 | 17597.0709 | 0.0272 |
| 9 | 0 | 9 | 8 | ← | 8 | 0 | 8 | 7 | 18088.4965 | 0.0176 |
| 9 | 0 | 9 | 9 | ← | 8 | 0 | 8 | 8 | 18088.4965 | 0.0003 |
| 9 | 0 | 9 | 10 | ← | 8 | 0 | 8 | 9 | 18088.4965 | -0.0002 |
| 6 | 2 | 5 | 6 | ← | 5 | 1 | 4 | 5 | 18124.2867 | 0.0172 |
| 7 | 1 | 6 | 7 | ← | 6 | 0 | 6 | 6 | 18308.0370 | 0.0269 |
| 9 | 2 | 8 | 8 | ← | 8 | 2 | 7 | 7 | 18430.6164 | 0.0027 |
| 9 | 2 | 8 | 10 | ← | 8 | 2 | 7 | 9 | 18430.6164 | -0.0072 |
| 9 | 7 | 3 | 9 | ← | 8 | 7 | 2 | 8 | 18521.7564 | -0.0077 |
| 9 | 6 | 4 | 9 | ← | 8 | 6 | 3 | 8 | 18525.7764 | 0.0145 |
| 9 | 6 | 3 | 9 | ← | 8 | 6 | 2 | 8 | 18525.7764 | 0.0143 |
| 9 | 6 | 4 | 8 | ← | 8 | 6 | 3 | 7 | 18526.1984 | -0.0084 |
| 9 | 6 | 3 | 8 | ← | 8 | 6 | 2 | 7 | 18526.1984 | -0.0086 |
| 9 | 5 | 5 | 9 | ← | 8 | 5 | 4 | 8 | 18532.4848 | 0.0161 |
| 9 | 5 | 4 | 9 | ← | 8 | 5 | 3 | 8 | 18532.4848 | -0.0080 |
| 9 | 5 | 4 | 10 | ← | 8 | 5 | 3 | 9 | 18532.7818 | 0.0142 |
| 9 | 5 | 5 | 8 | ← | 8 | 5 | 4 | 9 | 18532.7818 | 0.0134 |
| 9 | 5 | 5 | 8 | ← | 8 | 5 | 4 | 7 | 18532.7818 | 0.0070 |
| 9 | 5 | 4 | 8 | ← | 8 | 5 | 3 | 9 | 18532.7818 | -0.0107 |
| 9 | 5 | 4 | 8 | ← | 8 | 5 | 3 | 7 | 18532.7818 | -0.0171 |
| 9 | 4 | 6 | 10 | ← | 8 | 4 | 5 | 9 | 18544.7217 | -0.0134 |
| 9 | 4 | 6 | 8 | ← | 8 | 4 | 5 | 7 | 18544.7217 | -0.0271 |
| 9 | 4 | 5 | 10 | ← | 8 | 4 | 4 | 9 | 18546.2137 | -0.0288 |
| 9 | 1 | 9 | 10 | ← | 8 | 0 | 8 | 9 | 18748.5979 | 0.0098 |
| 9 | 1 | 9 | 9 | ← | 8 | 0 | 8 | 8 | 18748.5979 | -0.0279 |
| 9 | 2 | 7 | 8 | ← | 8 | 2 | 6 | 7 | 18845.7535 | 0.0106 |
| 9 | 2 | 7 | 10 | ← | 8 | 2 | 6 | 9 | 18845.7535 | 0.0007 |
| 9 | 1 | 8 | 8 | ← | 8 | 1 | 7 | 7 | 18860.5112 | 0.0134 |
| 9 | 1 | 8 | 9 | ← | 8 | 1 | 7 | 8 | 18860.5112 | 0.0103 |
| 9 | 1 | 8 | 10 | ← | 8 | 1 | 7 | 9 | 18860.5112 | -0.0030 |
| 4 | 3 | 2 | 5 | ← | 3 | 2 | 1 | 4 | 19246.7188 | 0.0152 |
| 4 | 3 | 2 | 4 | ← | 3 | 2 | 1 | 3 | 19247.1714 | 0.0237 |
| 4 | 3 | 1 | 5 | ← | 3 | 2 | 1 | 4 | 19247.3757 | -0.0162 |
| 4 | 3 | 1 | 4 | ← | 3 | 2 | 1 | 3 | 19247.8690 | 0.0331 |
| 4 | 3 | 2 | 5 | ← | 3 | 2 | 2 | 4 | 19267.5596 | 0.0074 |
| 4 | 3 | 1 | 4 | ← | 3 | 2 | 2 | 3 | 19268.6969 | 0.0187 |
| 4 | 3 | 1 | 4 | ← | 3 | 2 | 2 | 4 | 19268.6969 | 0.0186 |
| 10 | 0 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 19368.8165 | 0.0284 |
| 10 | 0 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 19368.8165 | -0.0002 |
| 10 | 0 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 19368.8165 | -0.0103 |
| 9 | 5 | 4 | 10 | ← | 9 | 4 | 5 | 10 | 19816.5015 | -0.0127 |
| 9 | 5 | 4 | 9 | ← | 9 | 4 | 5 | 9 | 19816.9384 | 0.0274 |
| 9 | 5 | 5 | 10 | ← | 9 | 4 | 6 | 10 | 19818.9501 | 0.0153 |

| J' | $K_{a'}$ | $K_{c'}$ | F' | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | 5 | 3 | 8 | ← | 8 | 4 | 4 | 7 | 19829.9673 | -0.0182 |
| 8 | 5 | 3 | 9 | ← | 8 | 4 | 4 | 9 | 19829.9673 | -0.0219 |
| 8 | 5 | 3 | 8 | ← | 8 | 4 | 4 | 8 | 19830.4764 | -0.0053 |
| 7 | 5 | 3 | 6 | ← | 7 | 4 | 4 | 6 | 19839.4154 | -0.0030 |
| 7 | 2 | 6 | 6 | ← | 6 | 1 | 5 | 7 | 19851.5048 | 0.0263 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 19874.8534 | 0.0093 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 19874.8534 | 0.0080 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 19874.8534 | -0.0034 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 20028.9178 | 0.0138 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 20028.9178 | 0.0000 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 20028.9178 | -0.0004 |
| 10 | 2 | 9 | 10 | ← | 9 | 2 | 8 | 9 | 20457.0110 | 0.0259 |
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 8 | 20457.0110 | 0.0004 |
| 10 | 2 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 20457.0110 | -0.0088 |
| 10 | 1 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 20534.9537 | 0.0224 |
| 10 | 1 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 20534.9537 | 0.0054 |
| 10 | 1 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 20534.9537 | -0.0214 |
| 10 | 7 | 4 | 10 | ← | 9 | 7 | 3 | 9 | 20582.5930 | 0.0102 |
| 10 | 7 | 3 | 11 | ← | 9 | 7 | 2 | 10 | 20582.9882 | 0.0159 |
| 10 | 7 | 4 | 11 | ← | 9 | 7 | 3 | 10 | 20582.9882 | 0.0159 |
| 10 | 7 | 3 | 9 | ← | 9 | 7 | 2 | 8 | 20582.9882 | -0.0325 |
| 10 | 6 | 5 | 10 | ← | 9 | 6 | 4 | 9 | 20588.0159 | 0.0023 |
| 10 | 6 | 4 | 10 | ← | 9 | 6 | 3 | 9 | 20588.0159 | 0.0015 |
| 10 | 6 | 5 | 11 | ← | 9 | 6 | 4 | 10 | 20588.3265 | 0.0250 |
| 10 | 6 | 4 | 11 | ← | 9 | 6 | 3 | 10 | 20588.3265 | 0.0242 |
| 10 | 6 | 5 | 9 | ← | 9 | 6 | 4 | 10 | 20588.3265 | 0.0222 |
| 10 | 6 | 4 | 9 | ← | 9 | 6 | 3 | 10 | 20588.3265 | 0.0214 |
| 10 | 5 | 6 | 9 | ← | 9 | 5 | 5 | 8 | 20597.3770 | -0.0049 |
| 10 | 5 | 6 | 9 | ← | 9 | 5 | 5 | 10 | 20597.3770 | -0.0299 |
| 10 | 4 | 7 | 11 | ← | 9 | 4 | 6 | 10 | 20613.3315 | -0.0067 |
| 10 | 4 | 7 | 9 | ← | 9 | 4 | 6 | 8 | 20613.3315 | -0.0129 |
| 10 | 4 | 6 | 11 | ← | 9 | 4 | 5 | 10 | 20616.5813 | -0.0046 |
| 10 | 4 | 6 | 9 | ← | 9 | 4 | 5 | 8 | 20616.5813 | -0.0109 |
| 10 | 1 | 9 | 9 | ← | 9 | 1 | 8 | 8 | 20909.6826 | 0.0097 |
| 10 | 1 | 9 | 10 | ← | 9 | 1 | 8 | 9 | 20909.6826 | 0.0046 |
| 10 | 1 | 9 | 11 | ← | 9 | 1 | 8 | 10 | 20909.6826 | -0.0039 |
| 10 | 2 | 8 | 10 | ← | 9 | 2 | 7 | 9 | 20986.0342 | 0.0305 |
| 10 | 2 | 8 | 9 | ← | 9 | 2 | 7 | 8 | 20986.0342 | -0.0001 |
| 10 | 2 | 8 | 11 | ← | 9 | 2 | 7 | 10 | 20986.0342 | -0.0094 |
| 5 | 3 | 3 | 6 | ← | 4 | 2 | 2 | 5 | 21278.0579 | 0.0090 |
| 5 | 3 | 3 | 4 | ← | 4 | 2 | 2 | 5 | 21278.0579 | -0.0177 |
| 5 | 3 | 3 | 5 | ← | 4 | 2 | 2 | 4 | 21278.4409 | 0.0090 |
| 5 | 3 | 2 | 6 | ← | 4 | 2 | 3 | 5 | 21343.0878 | 0.0227 |
| 5 | 3 | 2 | 5 | ← | 4 | 2 | 3 | 4 | 21343.4494 | 0.0133 |
| 11 | 0 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 21458.3973 | 0.0178 |
| 11 | 0 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 21458.3973 | -0.0010 |
| 11 | 0 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 21458.3973 | -0.0099 |
| 11 | 1 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 21838.9148 | 0.0066 |
| 11 | 1 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 21838.9148 | 0.0047 |
| 11 | 1 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 21838.9148 | -0.0039 |
| 11 | 0 | 11 | 10 | ← | 10 | 0 | 10 | 9 | 21964.4339 | 0.0083 |
| 11 | 0 | 11 | 11 | ← | 10 | 0 | 10 | 10 | 21964.4339 | -0.0027 |
| 11 | 0 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 21964.4339 | -0.0033 |
| 7 | 2 | 6 | 7 | ← | 6 | 1 | 6 | 6 | 22171.8556 | -0.0184 |
| 7 | 2 | 6 | 6 | ← | 6 | 1 | 6 | 7 | 22171.8556 | -0.0186 |
| 11 | 1 | 11 | 10 | ← | 10 | 0 | 10 | 9 | 22344.9474 | 0.0119 |
| 11 | 1 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 22344.9474 | -0.0014 |
| 11 | 1 | 11 | 11 | ← | 10 | 0 | 10 | 10 | 22344.9474 | -0.0199 |
| 11 | 2 | 10 | 11 | ← | 10 | 2 | 9 | 10 | 22477.0352 | 0.0178 |
| 11 | 2 | 10 | 10 | ← | 10 | 2 | 9 | 9 | 22477.0352 | 0.0001 |
| 11 | 2 | 10 | 12 | ← | 10 | 2 | 9 | 11 | 22477.0352 | -0.0082 |
| 11 | 7 | 4 | 11 | ← | 10 | 7 | 3 | 10 | 22644.2109 | -0.0098 |
| 11 | 7 | 5 | 11 | ← | 10 | 7 | 4 | 10 | 22644.2109 | -0.0098 |
| 11 | 7 | 4 | 10 | ← | 10 | 7 | 3 | 9 | 22644.5518 | 0.0056 |
| 11 | 7 | 5 | 10 | ← | 10 | 7 | 4 | 9 | 22644.5518 | 0.0057 |
| 11 | 6 | 6 | 12 | ← | 10 | 6 | 5 | 11 | 22651.6102 | -0.0283 |
| 11 | 6 | 5 | 12 | ← | 10 | 6 | 4 | 11 | 22651.6102 | -0.0307 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | 5 | 7 | 12 | ← | 10 | 5 | 6 | 11 | 22663.7005 | -0.0063 |
| 11 | 5 | 7 | 10 | ← | 10 | 5 | 6 | 9 | 22663.7005 | -0.0164 |
| 11 | 5 | 6 | 11 | ← | 10 | 5 | 5 | 10 | 22663.7005 | -0.0215 |
| 11 | 5 | 6 | 10 | ← | 10 | 5 | 5 | 11 | 22663.9370 | 0.0089 |
| 7 | 2 | 5 | 6 | ← | 6 | 1 | 6 | 5 | 22672.2162 | 0.0344 |
| 7 | 2 | 5 | 8 | ← | 6 | 1 | 6 | 7 | 22672.2162 | -0.0107 |
| 11 | 4 | 8 | 10 | ← | 10 | 4 | 7 | 9 | 22684.1422 | 0.0384 |
| 11 | 3 | 9 | 10 | ← | 10 | 3 | 8 | 9 | 22685.3736 | 0.0020 |
| 11 | 3 | 9 | 12 | ← | 10 | 3 | 8 | 11 | 22685.3736 | -0.0019 |
| 11 | 4 | 7 | 12 | ← | 10 | 4 | 6 | 11 | 22690.5761 | 0.0284 |
| 11 | 4 | 7 | 10 | ← | 10 | 4 | 6 | 9 | 22690.5761 | 0.0262 |
| 11 | 3 | 8 | 10 | ← | 10 | 3 | 7 | 9 | 22802.1755 | 0.0321 |
| 11 | 3 | 8 | 12 | ← | 10 | 3 | 7 | 11 | 22802.1755 | 0.0284 |
| 11 | 1 | 10 | 10 | ← | 10 | 1 | 9 | 9 | 22941.5203 | 0.0044 |
| 11 | 1 | 10 | 11 | ← | 10 | 1 | 9 | 10 | 22941.5203 | -0.0021 |
| 11 | 1 | 10 | 12 | ← | 10 | 1 | 9 | 11 | 22941.5203 | -0.0070 |
| 11 | 2 | 9 | 11 | ← | 10 | 2 | 8 | 10 | 23123.3653 | 0.0108 |
| 11 | 2 | 9 | 10 | ← | 10 | 2 | 8 | 9 | 23123.3653 | -0.0105 |
| 11 | 2 | 9 | 12 | ← | 10 | 2 | 8 | 11 | 23123.3653 | -0.0190 |
| 9 | 2 | 8 | 10 | ← | 8 | 1 | 7 | 9 | 23163.9380 | 0.0210 |
| 6 | 3 | 4 | 6 | ← | 5 | 2 | 3 | 5 | 23282.3245 | 0.0097 |
| 6 | 3 | 3 | 6 | ← | 5 | 2 | 3 | 5 | 23290.5442 | 0.0049 |
| 6 | 3 | 3 | 7 | ← | 5 | 2 | 4 | 6 | 23434.3003 | 0.0191 |
| 6 | 3 | 3 | 6 | ← | 5 | 2 | 4 | 5 | 23434.5945 | 0.0151 |
| 6 | 3 | 3 | 5 | ← | 5 | 2 | 4 | 5 | 23435.0971 | -0.0267 |
| 12 | 0 | 12 | 12 | ← | 11 | 1 | 11 | 11 | 23517.7123 | 0.0055 |
| 12 | 0 | 12 | 11 | ← | 11 | 1 | 11 | 10 | 23517.7123 | -0.0065 |
| 12 | 0 | 12 | 13 | ← | 11 | 1 | 11 | 12 | 23517.7123 | -0.0144 |
| 4 | 4 | 1 | 3 | ← | 3 | 3 | 0 | 3 | 23668.3353 | -0.0248 |
| 4 | 4 | 1 | 3 | ← | 3 | 3 | 0 | 2 | 23670.4656 | 0.0334 |
| 4 | 4 | 0 | 5 | ← | 3 | 3 | 1 | 4 | 23670.4656 | 0.0181 |
| 12 | 1 | 12 | 11 | ← | 11 | 1 | 11 | 10 | 23799.2033 | -0.0007 |
| 12 | 1 | 12 | 12 | ← | 11 | 1 | 11 | 11 | 23799.2033 | -0.0030 |
| 12 | 1 | 12 | 13 | ← | 11 | 1 | 11 | 12 | 23799.2033 | -0.0098 |
| 12 | 0 | 12 | 11 | ← | 11 | 0 | 11 | 10 | 23898.2291 | 0.0004 |
| 12 | 0 | 12 | 12 | ← | 11 | 0 | 11 | 11 | 23898.2291 | -0.0082 |
| 12 | 0 | 12 | 13 | ← | 11 | 0 | 11 | 12 | 23898.2291 | -0.0091 |
| 12 | 1 | 12 | 11 | ← | 11 | 0 | 11 | 10 | 24179.7269 | 0.0130 |
| 12 | 1 | 12 | 13 | ← | 11 | 0 | 11 | 12 | 24179.7269 | 0.0022 |
| 12 | 1 | 12 | 12 | ← | 11 | 0 | 11 | 11 | 24179.7269 | -0.0101 |
| 8 | 6 | 2 | 7 | ← | 8 | 5 | 3 | 8 | 24252.4494 | 0.0012 |
| 8 | 6 | 3 | 7 | ← | 8 | 5 | 4 | 8 | 24252.4494 | -0.0084 |
| 12 | 2 | 11 | 12 | ← | 11 | 2 | 10 | 11 | 24490.3239 | -0.0027 |
| 12 | 2 | 11 | 11 | ← | 11 | 2 | 10 | 10 | 24490.3239 | -0.0150 |
| 12 | 2 | 11 | 13 | ← | 11 | 2 | 10 | 12 | 24490.3239 | -0.0225 |
| 12 | 3 | 10 | 12 | ← | 11 | 3 | 9 | 11 | 24748.5490 | 0.0033 |
| 12 | 4 | 9 | 11 | ← | 11 | 4 | 8 | 10 | 24756.9450 | -0.0016 |
| 12 | 4 | 9 | 13 | ← | 11 | 4 | 8 | 12 | 24756.9450 | -0.0017 |
| 10 | 2 | 9 | 9 | ← | 9 | 1 | 8 | 8 | 24760.3959 | -0.0003 |
| 10 | 2 | 9 | 11 | ← | 9 | 1 | 8 | 10 | 24760.3959 | -0.0265 |
| 12 | 4 | 8 | 11 | ← | 11 | 4 | 7 | 10 | 24768.9007 | -0.0105 |
| 12 | 4 | 8 | 13 | ← | 11 | 4 | 7 | 12 | 24768.9007 | -0.0105 |
| 12 | 3 | 9 | 11 | ← | 11 | 3 | 8 | 10 | 24923.7328 | -0.0029 |
| 12 | 3 | 9 | 13 | ← | 11 | 3 | 8 | 12 | 24923.7328 | -0.0070 |
| 12 | 1 | 11 | 11 | ← | 11 | 1 | 10 | 10 | 24954.0279 | -0.0097 |
| 12 | 1 | 11 | 12 | ← | 11 | 1 | 10 | 11 | 24954.0279 | -0.0173 |
| 12 | 1 | 11 | 13 | ← | 11 | 1 | 10 | 12 | 24954.0279 | -0.0195 |
| 7 | 3 | 5 | 8 | ← | 6 | 2 | 4 | 7 | 25245.7166 | 0.0117 |
| 7 | 3 | 5 | 7 | ← | 6 | 2 | 4 | 6 | 25245.9891 | 0.0191 |
| 12 | 2 | 10 | 12 | ← | 11 | 2 | 9 | 11 | 25253.3477 | -0.0063 |
| 8 | 2 | 6 | 7 | ← | 7 | 1 | 7 | 6 | 25423.8955 | 0.0196 |
| 8 | 2 | 6 | 9 | ← | 7 | 1 | 7 | 8 | 25423.8955 | -0.0113 |
| 7 | 3 | 4 | 8 | ← | 6 | 2 | 5 | 7 | 25550.2286 | -0.0070 |
| 7 | 3 | 4 | 7 | ← | 6 | 2 | 5 | 6 | 25550.4871 | 0.0133 |
| 13 | 0 | 13 | 12 | ← | 12 | 1 | 12 | 11 | 25550.8671 | 0.0113 |
| 13 | 0 | 13 | 12 | ← | 12 | 0 | 12 | 11 | 25832.3418 | 0.0007 |
| 13 | 0 | 13 | 13 | ← | 12 | 0 | 12 | 12 | 25832.3418 | -0.0061 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | 0 | 13 | 14 | ← | 12 | 0 | 12 | 13 | 25832.3418 | -0.0073 |
| | | | | | | | | | RMS | 11.0 kHz |

Table S13 Linelist for Conformer V of isoleucinol. OMC is the difference between the observed and calculated transition.

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 1 | 2 | 2 | ← | 3 | 0 | 3 | 2 | 2095.3002 | 0.0142 |
| 3 | 1 | 2 | 4 | ← | 3 | 0 | 3 | 4 | 2095.4377 | 0.0027 |
| 3 | 1 | 2 | 3 | ← | 3 | 0 | 3 | 3 | 2095.8606 | -0.0003 |
| 1 | 0 | 1 | 1 | ← | 0 | 0 | 0 | 1 | 2477.2733 | -0.0106 |
| 4 | 2 | 2 | 4 | ← | 4 | 1 | 3 | 4 | 2759.9877 | -0.0010 |
| 3 | 2 | 1 | 2 | ← | 3 | 1 | 2 | 2 | 2819.9531 | 0.0030 |
| 3 | 2 | 1 | 4 | ← | 3 | 1 | 2 | 4 | 2820.1799 | 0.0019 |
| 3 | 2 | 1 | 3 | ← | 3 | 1 | 2 | 3 | 2820.8300 | 0.0006 |
| 4 | 1 | 3 | 5 | ← | 4 | 0 | 4 | 5 | 2905.4132 | 0.0017 |
| 4 | 1 | 3 | 4 | ← | 4 | 0 | 4 | 4 | 2905.7628 | 0.0028 |
| 2 | 2 | 0 | 3 | ← | 2 | 1 | 1 | 3 | 3007.8292 | 0.0021 |
| 2 | 2 | 0 | 2 | ← | 2 | 1 | 1 | 2 | 3009.1702 | 0.0047 |
| 1 | 1 | 1 | 2 | ← | 0 | 0 | 0 | 1 | 3465.4393 | 0.0008 |
| 1 | 1 | 1 | 1 | ← | 0 | 0 | 0 | 1 | 3465.7676 | 0.0037 |
| 1 | 1 | 0 | 2 | ← | 0 | 0 | 0 | 1 | 3728.0622 | 0.0090 |
| 1 | 1 | 0 | 1 | ← | 0 | 0 | 0 | 1 | 3728.6377 | -0.0017 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 4 | 4170.5699 | 0.0042 |
| 2 | 1 | 2 | 2 | ← | 1 | 1 | 1 | 1 | 4692.6683 | 0.0000 |
| 2 | 1 | 2 | 2 | ← | 1 | 1 | 1 | 2 | 4692.9967 | 0.0030 |
| 2 | 1 | 2 | 3 | ← | 1 | 1 | 1 | 2 | 4693.6134 | -0.0085 |
| 2 | 1 | 2 | 1 | ← | 1 | 1 | 1 | 0 | 4694.4540 | -0.0054 |
| 4 | 2 | 3 | 3 | ← | 4 | 1 | 4 | 3 | 4738.1959 | 0.0067 |
| 4 | 2 | 3 | 5 | ← | 4 | 1 | 4 | 5 | 4738.3470 | -0.0017 |
| 4 | 2 | 3 | 4 | ← | 4 | 1 | 4 | 4 | 4738.9613 | -0.0083 |
| 2 | 0 | 2 | 2 | ← | 1 | 0 | 1 | 2 | 4909.3738 | -0.0023 |
| 2 | 0 | 2 | 1 | ← | 1 | 0 | 1 | 0 | 4909.5498 | 0.0019 |
| 2 | 0 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 4910.3651 | -0.0007 |
| 2 | 0 | 2 | 1 | ← | 1 | 0 | 1 | 1 | 4911.8348 | 0.0071 |
| 4 | 3 | 1 | 3 | ← | 4 | 2 | 2 | 3 | 5156.3598 | -0.0025 |
| 4 | 3 | 1 | 5 | ← | 4 | 2 | 2 | 5 | 5156.5504 | -0.0011 |
| 4 | 3 | 1 | 4 | ← | 4 | 2 | 2 | 4 | 5157.2835 | -0.0034 |
| 2 | 1 | 1 | 2 | ← | 1 | 1 | 0 | 1 | 5217.9732 | -0.0013 |
| 2 | 1 | 1 | 3 | ← | 1 | 1 | 0 | 2 | 5218.9061 | -0.0034 |
| 2 | 1 | 1 | 1 | ← | 1 | 1 | 0 | 0 | 5219.9784 | -0.0047 |
| 3 | 3 | 0 | 2 | ← | 3 | 2 | 1 | 2 | 5404.3099 | 0.0028 |
| 3 | 3 | 0 | 4 | ← | 3 | 2 | 1 | 4 | 5404.7414 | 0.0005 |
| 3 | 3 | 0 | 3 | ← | 3 | 2 | 1 | 3 | 5405.9820 | 0.0022 |
| 3 | 3 | 1 | 2 | ← | 3 | 2 | 2 | 2 | 5619.5739 | -0.0043 |
| 3 | 3 | 1 | 2 | ← | 3 | 2 | 2 | 3 | 5619.5739 | -0.0045 |
| 3 | 3 | 1 | 4 | ← | 3 | 2 | 2 | 3 | 5620.0245 | 0.0013 |
| 3 | 3 | 1 | 4 | ← | 3 | 2 | 2 | 4 | 5620.0245 | 0.0013 |
| 3 | 3 | 1 | 3 | ← | 3 | 2 | 2 | 2 | 5621.2938 | 0.0004 |
| 3 | 3 | 1 | 3 | ← | 3 | 2 | 2 | 3 | 5621.2938 | 0.0003 |
| 2 | 1 | 2 | 1 | ← | 1 | 0 | 1 | 0 | 5679.8469 | 0.0010 |
| 2 | 1 | 2 | 2 | ← | 1 | 0 | 1 | 2 | 5680.2394 | 0.0030 |
| 2 | 1 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 5680.8623 | -0.0022 |
| 2 | 1 | 2 | 2 | ← | 1 | 0 | 1 | 1 | 5681.1389 | -0.0092 |
| 4 | 3 | 2 | 5 | ← | 4 | 2 | 3 | 5 | 5734.3324 | 0.0007 |
| 4 | 3 | 2 | 4 | ← | 4 | 2 | 3 | 4 | 5735.1210 | -0.0004 |
| 3 | 0 | 3 | 3 | ← | 2 | 1 | 2 | 3 | 6488.0016 | 0.0112 |
| 3 | 0 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 6488.6176 | -0.0009 |
| 3 | 0 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 6489.0297 | -0.0058 |
| 3 | 0 | 3 | 2 | ← | 2 | 1 | 2 | 2 | 6490.0175 | -0.0122 |
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 3 | 7012.8115 | -0.0023 |
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 7013.4394 | -0.0027 |
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 7013.7215 | -0.0010 |
| 3 | 1 | 3 | 2 | ← | 2 | 1 | 2 | 2 | 7014.6683 | -0.0007 |
| 3 | 0 | 3 | 3 | ← | 2 | 0 | 2 | 3 | 7258.4942 | 0.0050 |
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 1 | 7259.3566 | 0.0062 |
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 7259.5341 | -0.0002 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 2 | 7260.9045 | 0.0145 |
| 3 | 2 | 2 | 3 | ← | 2 | 2 | 1 | 2 | 7433.3599 | 0.0030 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 2 | 7433.3599 | 0.0028 |
| 3 | 2 | 2 | 4 | ← | 2 | 2 | 1 | 3 | 7434.3311 | -0.0026 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 1 | 7434.8750 | -0.0017 |
| 3 | 2 | 1 | 3 | ← | 2 | 2 | 0 | 2 | 7607.9581 | -0.0035 |
| 3 | 2 | 1 | 2 | ← | 2 | 2 | 0 | 3 | 7608.9147 | 0.0065 |
| 3 | 2 | 1 | 4 | ← | 2 | 2 | 0 | 3 | 7608.9147 | -0.0044 |
| 3 | 2 | 1 | 2 | ← | 2 | 2 | 0 | 1 | 7609.4552 | -0.0027 |
| 4 | 1 | 3 | 5 | ← | 3 | 2 | 2 | 4 | 7729.4308 | -0.0070 |
| 4 | 1 | 3 | 3 | ← | 3 | 2 | 2 | 2 | 7729.6190 | -0.0101 |
| 4 | 1 | 3 | 3 | ← | 3 | 2 | 2 | 3 | 7729.6190 | -0.0103 |
| 4 | 1 | 3 | 3 | ← | 3 | 2 | 2 | 4 | 7729.6190 | -0.0103 |
| 5 | 4 | 2 | 4 | ← | 5 | 3 | 3 | 4 | 7752.0904 | -0.0022 |
| 5 | 4 | 2 | 6 | ← | 5 | 3 | 3 | 6 | 7752.2381 | -0.0035 |
| 5 | 4 | 2 | 5 | ← | 5 | 3 | 3 | 5 | 7752.9692 | -0.0033 |
| 4 | 4 | 1 | 3 | ← | 4 | 3 | 2 | 3 | 7761.8329 | -0.0057 |
| 4 | 4 | 1 | 5 | ← | 4 | 3 | 2 | 5 | 7762.1130 | -0.0039 |
| 4 | 4 | 1 | 4 | ← | 4 | 3 | 2 | 4 | 7763.1896 | -0.0089 |
| 6 | 4 | 3 | 5 | ← | 6 | 3 | 4 | 5 | 7766.6277 | -0.0057 |
| 6 | 4 | 3 | 7 | ← | 6 | 3 | 4 | 7 | 7766.7180 | -0.0045 |
| 6 | 4 | 3 | 6 | ← | 6 | 3 | 4 | 6 | 7767.2442 | -0.0058 |
| 3 | 1 | 3 | 3 | ← | 2 | 0 | 2 | 3 | 7783.3108 | -0.0018 |
| 3 | 1 | 3 | 2 | ← | 2 | 0 | 2 | 1 | 7783.9902 | 0.0006 |
| 3 | 1 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 7784.2199 | -0.0014 |
| 3 | 1 | 3 | 3 | ← | 2 | 0 | 2 | 2 | 7784.3053 | 0.0029 |
| 3 | 1 | 3 | 2 | ← | 2 | 0 | 2 | 2 | 7785.5246 | -0.0045 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 3 | 7795.9520 | 0.0030 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 7796.2982 | 0.0005 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 7796.5622 | -0.0060 |
| 3 | 1 | 2 | 2 | ← | 2 | 1 | 1 | 2 | 7797.1347 | 0.0007 |
| 2 | 2 | 1 | 1 | ← | 1 | 1 | 0 | 1 | 8179.8449 | 0.0123 |
| 2 | 2 | 1 | 3 | ← | 1 | 1 | 0 | 2 | 8180.9724 | 0.0107 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 0 | 1 | 8181.3496 | -0.0028 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 0 | 2 | 8181.9518 | 0.0131 |
| 2 | 2 | 0 | 1 | ← | 1 | 1 | 0 | 1 | 8225.5841 | -0.0166 |
| 2 | 2 | 0 | 3 | ← | 1 | 1 | 0 | 2 | 8226.7287 | -0.0079 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 0 | 1 | 8227.1147 | -0.0252 |
| 2 | 2 | 1 | 1 | ← | 1 | 1 | 1 | 1 | 8442.7162 | 0.0080 |
| 2 | 2 | 1 | 3 | ← | 1 | 1 | 1 | 2 | 8443.5738 | -0.0025 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 1 | 1 | 8444.2311 | 0.0031 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 1 | 2 | 8444.5520 | -0.0013 |
| 2 | 2 | 0 | 1 | ← | 1 | 1 | 1 | 1 | 8488.4731 | -0.0031 |
| 2 | 2 | 0 | 3 | ← | 1 | 1 | 1 | 2 | 8489.3456 | -0.0057 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 1 | 1 | 8490.0176 | 0.0020 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 1 | 2 | 8490.3439 | 0.0029 |
| 4 | 0 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 8994.4254 | 0.0175 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 9308.4279 | -0.0081 |
| 3 | 1 | 2 | 2 | ← | 2 | 0 | 2 | 1 | 9354.6288 | -0.0075 |
| 3 | 1 | 2 | 4 | ← | 2 | 0 | 2 | 3 | 9354.9663 | -0.0031 |
| 3 | 1 | 2 | 3 | ← | 2 | 0 | 2 | 2 | 9355.3328 | -0.0068 |
| 4 | 0 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 9519.2755 | -0.0034 |
| 4 | 0 | 4 | 3 | ← | 3 | 0 | 3 | 3 | 9520.6099 | 0.0045 |
| 4 | 1 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 9833.2629 | 0.0099 |
| 4 | 1 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 9833.2629 | 0.0032 |
| 4 | 1 | 4 | 3 | ← | 3 | 0 | 3 | 3 | 9834.5616 | -0.0037 |
| 4 | 2 | 3 | 4 | ← | 3 | 2 | 2 | 3 | 9875.9176 | -0.0138 |
| 4 | 2 | 3 | 4 | ← | 3 | 2 | 2 | 4 | 9875.9176 | -0.0139 |
| 4 | 2 | 3 | 5 | ← | 3 | 2 | 2 | 4 | 9876.3273 | -0.0218 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 2 | 9876.4561 | -0.0003 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 3 | 9876.4561 | -0.0005 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 4 | 9876.4561 | -0.0005 |
| 4 | 3 | 2 | 3 | ← | 3 | 3 | 1 | 3 | 9989.3051 | 0.0134 |
| 4 | 3 | 2 | 4 | ← | 3 | 3 | 1 | 3 | 9989.7399 | -0.0195 |
| 4 | 3 | 2 | 5 | ← | 3 | 3 | 1 | 4 | 9990.6416 | -0.0159 |
| 4 | 3 | 2 | 3 | ← | 3 | 3 | 1 | 2 | 9990.9978 | -0.0088 |
| 4 | 3 | 1 | 4 | ← | 3 | 3 | 0 | 3 | 10019.5911 | -0.0059 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | 3 | 1 | 5 | ← | 3 | 3 | 0 | 4 | 10020.4902 | -0.0034 |
| 4 | 2 | 2 | 4 | ← | 3 | 2 | 1 | 3 | 10268.2852 | -0.0046 |
| 4 | 2 | 2 | 5 | ← | 3 | 2 | 1 | 4 | 10268.6725 | -0.0104 |
| 4 | 2 | 2 | 3 | ← | 3 | 2 | 1 | 2 | 10268.8002 | 0.0131 |
| 4 | 1 | 3 | 4 | ← | 3 | 1 | 2 | 4 | 10328.4969 | -0.0142 |
| 4 | 1 | 3 | 4 | ← | 3 | 1 | 2 | 3 | 10329.1241 | -0.0063 |
| 4 | 1 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 10329.2674 | 0.0120 |
| 4 | 1 | 3 | 3 | ← | 3 | 1 | 2 | 3 | 10330.0747 | 0.0084 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 1 | 10396.1896 | -0.0023 |
| 3 | 2 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 10396.3845 | -0.0013 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 1 | 3 | 10396.3845 | -0.0013 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 3 | 10396.3845 | -0.0015 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 10396.7340 | -0.0006 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 2 | 10396.7340 | -0.0008 |
| 3 | 2 | 1 | 2 | ← | 2 | 1 | 1 | 1 | 10616.5382 | -0.0029 |
| 3 | 2 | 1 | 2 | ← | 2 | 1 | 1 | 3 | 10616.7457 | 0.0103 |
| 3 | 2 | 1 | 4 | ← | 2 | 1 | 1 | 3 | 10616.7457 | -0.0006 |
| 3 | 2 | 1 | 3 | ← | 2 | 1 | 1 | 2 | 10617.1353 | 0.0083 |
| 5 | 1 | 4 | 5 | ← | 4 | 2 | 3 | 4 | 10644.5274 | -0.0067 |
| 5 | 1 | 4 | 6 | ← | 4 | 2 | 3 | 5 | 10644.9423 | 0.0072 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 2 | 1 | 11183.9304 | -0.0086 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 2 | 3 | 11184.2837 | -0.0044 |
| 3 | 2 | 2 | 4 | ← | 2 | 1 | 2 | 3 | 11184.2837 | -0.0044 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 2 | 3 | 11184.2837 | -0.0046 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 2 | 2 | 11184.9202 | 0.0037 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 2 | 2 | 11184.9202 | 0.0035 |
| 3 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 1 | 11404.2883 | 0.0000 |
| 3 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 3 | 11404.6485 | 0.0109 |
| 3 | 2 | 1 | 4 | ← | 2 | 1 | 2 | 3 | 11404.6485 | 0.0000 |
| 3 | 2 | 1 | 3 | ← | 2 | 1 | 2 | 2 | 11405.3145 | 0.0056 |
| 5 | 0 | 5 | 5 | ← | 4 | 1 | 4 | 4 | 11409.1471 | 0.0252 |
| 5 | 1 | 5 | 4 | ← | 4 | 1 | 4 | 3 | 11578.5043 | 0.0071 |
| 5 | 0 | 5 | 4 | ← | 4 | 0 | 4 | 3 | 11723.1358 | -0.0068 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 11723.1358 | -0.0142 |
| 5 | 1 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 11892.5234 | 0.0121 |
| 5 | 2 | 4 | 5 | ← | 4 | 2 | 3 | 4 | 12288.4526 | -0.0087 |
| 5 | 2 | 4 | 6 | ← | 4 | 2 | 3 | 5 | 12288.6679 | -0.0153 |
| 4 | 2 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 12476.1609 | -0.0057 |
| 4 | 2 | 3 | 4 | ← | 3 | 1 | 2 | 3 | 12476.3576 | -0.0108 |
| 5 | 3 | 2 | 5 | ← | 4 | 3 | 1 | 4 | 12600.9659 | -0.0151 |
| 5 | 3 | 2 | 6 | ← | 4 | 3 | 1 | 5 | 12601.4439 | 0.0028 |
| 5 | 1 | 4 | 4 | ← | 4 | 1 | 3 | 3 | 12791.8235 | 0.0017 |
| 5 | 1 | 4 | 6 | ← | 4 | 1 | 3 | 5 | 12791.8235 | -0.0229 |
| 5 | 2 | 3 | 5 | ← | 4 | 2 | 2 | 4 | 12951.6056 | -0.0088 |
| 5 | 2 | 3 | 6 | ← | 4 | 2 | 2 | 5 | 12951.8040 | -0.0058 |
| 3 | 3 | 1 | 4 | ← | 2 | 2 | 0 | 3 | 13008.5593 | -0.0225 |
| 3 | 3 | 1 | 3 | ← | 2 | 2 | 0 | 2 | 13008.8519 | -0.0108 |
| 3 | 3 | 0 | 4 | ← | 2 | 2 | 0 | 3 | 13013.6421 | -0.0179 |
| 3 | 3 | 0 | 3 | ← | 2 | 2 | 0 | 2 | 13013.9530 | 0.0116 |
| 3 | 3 | 1 | 4 | ← | 2 | 2 | 1 | 3 | 13054.3497 | -0.0072 |
| 3 | 3 | 1 | 3 | ← | 2 | 2 | 1 | 2 | 13054.6404 | -0.0099 |
| 3 | 3 | 0 | 4 | ← | 2 | 2 | 1 | 3 | 13059.4400 | 0.0049 |
| 3 | 3 | 0 | 3 | ← | 2 | 2 | 1 | 2 | 13059.7371 | 0.0081 |
| 3 | 3 | 0 | 3 | ← | 2 | 2 | 1 | 3 | 13060.7053 | -0.0006 |
| 4 | 2 | 2 | 5 | ← | 3 | 1 | 2 | 4 | 13088.8392 | -0.0218 |
| 4 | 2 | 2 | 4 | ← | 3 | 1 | 2 | 3 | 13089.1148 | -0.0045 |
| 6 | 0 | 6 | 5 | ← | 5 | 1 | 5 | 4 | 13743.1308 | 0.0154 |
| 6 | 0 | 6 | 6 | ← | 5 | 0 | 5 | 5 | 13912.4182 | -0.0081 |
| 6 | 1 | 6 | 5 | ← | 5 | 0 | 5 | 4 | 13997.2337 | 0.0170 |
| 4 | 2 | 3 | 5 | ← | 3 | 1 | 3 | 4 | 14046.9031 | -0.0116 |
| 4 | 2 | 3 | 4 | ← | 3 | 1 | 3 | 3 | 14047.4131 | 0.0073 |
| 5 | 2 | 4 | 4 | ← | 4 | 1 | 3 | 3 | 14435.5534 | 0.0200 |
| 5 | 2 | 4 | 5 | ← | 4 | 1 | 3 | 4 | 14435.7002 | 0.0008 |
| 4 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 2 | 14659.3618 | -0.0219 |
| 4 | 2 | 2 | 5 | ← | 3 | 1 | 3 | 4 | 14659.6038 | -0.0052 |
| 4 | 2 | 2 | 4 | ← | 3 | 1 | 3 | 3 | 14660.1341 | -0.0225 |
| 6 | 2 | 5 | 6 | ← | 5 | 2 | 4 | 5 | 14666.1706 | -0.0121 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | 2 | 5 | 7 | ← | 5 | 2 | 4 | 6 | 14666.3159 | -0.0018 |
| 6 | 2 | 5 | 5 | ← | 5 | 2 | 4 | 4 | 14666.3159 | -0.0023 |
| 4 | 3 | 2 | 5 | ← | 3 | 2 | 1 | 4 | 15390.3085 | -0.0118 |
| 4 | 3 | 2 | 4 | ← | 3 | 2 | 1 | 3 | 15390.6591 | -0.0014 |
| 4 | 3 | 1 | 5 | ← | 3 | 2 | 1 | 4 | 15425.2174 | -0.0171 |
| 5 | 3 | 3 | 6 | ← | 4 | 2 | 2 | 5 | 17623.3325 | -0.0084 |
| 5 | 3 | 3 | 5 | ← | 4 | 2 | 2 | 4 | 17623.6191 | 0.0085 |
| 7 | 2 | 6 | 6 | ← | 6 | 1 | 5 | 5 | 18157.6706 | 0.0334 |
| 7 | 2 | 6 | 8 | ← | 6 | 1 | 5 | 7 | 18157.6706 | 0.0110 |
| 7 | 2 | 6 | 7 | ← | 6 | 1 | 5 | 6 | 18157.6706 | 0.0044 |
| 7 | 2 | 5 | 6 | ← | 6 | 2 | 4 | 5 | 18194.1068 | 0.0323 |
| 7 | 2 | 5 | 8 | ← | 6 | 2 | 4 | 7 | 18194.1068 | 0.0259 |
| 5 | 3 | 3 | 5 | ← | 4 | 2 | 3 | 4 | 18236.3600 | -0.0013 |
| 8 | 0 | 8 | 8 | ← | 7 | 1 | 7 | 7 | 18269.6051 | 0.0267 |
| 8 | 0 | 8 | 7 | ← | 7 | 1 | 7 | 6 | 18269.6051 | 0.0158 |
| 8 | 0 | 8 | 9 | ← | 7 | 1 | 7 | 8 | 18269.6051 | -0.0024 |
| 8 | 1 | 8 | 8 | ← | 7 | 1 | 7 | 7 | 18288.1235 | 0.0221 |
| 8 | 1 | 8 | 7 | ← | 7 | 1 | 7 | 6 | 18288.1235 | 0.0126 |
| 8 | 1 | 8 | 9 | ← | 7 | 1 | 7 | 8 | 18288.1235 | -0.0058 |
| 5 | 2 | 3 | 5 | ← | 4 | 1 | 4 | 4 | 18303.3663 | 0.0312 |
| 8 | 0 | 8 | 8 | ← | 7 | 0 | 7 | 7 | 18309.9524 | 0.0220 |
| 8 | 0 | 8 | 7 | ← | 7 | 0 | 7 | 6 | 18309.9524 | 0.0148 |
| 8 | 0 | 8 | 9 | ← | 7 | 0 | 7 | 8 | 18309.9524 | -0.0039 |
| 8 | 1 | 8 | 8 | ← | 7 | 0 | 7 | 7 | 18328.4745 | 0.0210 |
| 8 | 1 | 8 | 7 | ← | 7 | 0 | 7 | 6 | 18328.4745 | 0.0152 |
| 8 | 1 | 8 | 9 | ← | 7 | 0 | 7 | 8 | 18328.4745 | -0.0037 |
| 5 | 3 | 2 | 5 | ← | 4 | 2 | 3 | 4 | 18371.0258 | 0.0069 |
| 8 | 2 | 7 | 7 | ← | 7 | 2 | 6 | 6 | 19312.7513 | 0.0176 |
| 8 | 2 | 7 | 9 | ← | 7 | 2 | 6 | 8 | 19312.7513 | 0.0101 |
| 8 | 1 | 7 | 7 | ← | 7 | 1 | 6 | 6 | 19618.4324 | 0.0085 |
| 8 | 1 | 7 | 9 | ← | 7 | 1 | 6 | 8 | 19618.4324 | -0.0031 |
| 8 | 3 | 6 | 9 | ← | 7 | 3 | 5 | 8 | 19940.1128 | 0.0068 |
| 8 | 3 | 6 | 7 | ← | 7 | 3 | 5 | 6 | 19940.1128 | 0.0017 |
| 8 | 6 | 3 | 8 | ← | 7 | 6 | 2 | 7 | 19998.8349 | 0.0170 |
| 8 | 6 | 3 | 9 | ← | 7 | 6 | 2 | 8 | 19999.2878 | 0.0167 |
| 8 | 2 | 7 | 8 | ← | 7 | 1 | 6 | 7 | 20044.4772 | 0.0171 |
| 8 | 2 | 7 | 7 | ← | 7 | 1 | 6 | 6 | 20044.4772 | 0.0171 |
| 8 | 2 | 7 | 9 | ← | 7 | 1 | 6 | 8 | 20044.4772 | 0.0022 |
| 8 | 5 | 4 | 8 | ← | 7 | 5 | 3 | 7 | 20047.9802 | -0.0093 |
| 8 | 5 | 4 | 7 | ← | 7 | 5 | 3 | 8 | 20048.3130 | 0.0151 |
| 8 | 5 | 4 | 9 | ← | 7 | 5 | 3 | 8 | 20048.3130 | 0.0078 |
| 6 | 3 | 3 | 6 | ← | 5 | 2 | 3 | 5 | 20054.3467 | -0.0167 |
| 8 | 5 | 3 | 8 | ← | 7 | 5 | 2 | 7 | 20056.0208 | -0.0118 |
| 8 | 5 | 3 | 7 | ← | 7 | 5 | 2 | 8 | 20056.3582 | 0.0173 |
| 8 | 5 | 3 | 9 | ← | 7 | 5 | 2 | 8 | 20056.3582 | 0.0100 |
| 8 | 4 | 5 | 9 | ← | 7 | 4 | 4 | 8 | 20093.2746 | -0.0190 |
| 6 | 2 | 5 | 6 | ← | 5 | 1 | 5 | 5 | 20115.1664 | 0.0147 |
| 5 | 4 | 2 | 4 | ← | 4 | 3 | 1 | 3 | 20219.0255 | 0.0284 |
| 5 | 4 | 2 | 6 | ← | 4 | 3 | 1 | 5 | 20219.0255 | -0.0055 |
| 5 | 4 | 2 | 5 | ← | 4 | 3 | 1 | 4 | 20219.3111 | 0.0149 |
| 5 | 4 | 1 | 6 | ← | 4 | 3 | 1 | 5 | 20223.1683 | -0.0053 |
| 5 | 4 | 1 | 5 | ← | 4 | 3 | 1 | 4 | 20223.4570 | 0.0182 |
| 8 | 4 | 4 | 9 | ← | 7 | 4 | 3 | 8 | 20225.7222 | -0.0263 |
| 5 | 4 | 2 | 6 | ← | 4 | 3 | 2 | 5 | 20253.9431 | -0.0021 |
| 5 | 4 | 2 | 5 | ← | 4 | 3 | 2 | 4 | 20254.2308 | 0.0183 |
| 5 | 4 | 1 | 4 | ← | 4 | 3 | 2 | 3 | 20258.0836 | 0.0305 |
| 5 | 4 | 1 | 6 | ← | 4 | 3 | 2 | 5 | 20258.0836 | -0.0041 |
| 5 | 4 | 1 | 5 | ← | 4 | 3 | 2 | 4 | 20258.3701 | 0.0149 |
| 5 | 4 | 1 | 5 | ← | 4 | 3 | 2 | 5 | 20258.7562 | 0.0289 |
| 9 | 2 | 7 | 10 | ← | 8 | 3 | 6 | 9 | 20474.0332 | -0.0339 |
| 9 | 1 | 9 | 9 | ← | 8 | 1 | 8 | 8 | 20508.3663 | 0.0171 |
| 9 | 1 | 9 | 8 | ← | 8 | 1 | 8 | 7 | 20508.3663 | 0.0096 |
| 9 | 1 | 9 | 10 | ← | 8 | 1 | 8 | 9 | 20508.3663 | -0.0052 |
| 9 | 0 | 9 | 9 | ← | 8 | 0 | 8 | 8 | 20518.6107 | 0.0179 |
| 9 | 0 | 9 | 8 | ← | 8 | 0 | 8 | 7 | 20518.6107 | 0.0113 |
| 9 | 0 | 9 | 10 | ← | 8 | 0 | 8 | 9 | 20518.6107 | -0.0036 |
| 9 | 1 | 9 | 9 | ← | 8 | 0 | 8 | 8 | 20526.8868 | 0.0146 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | 1 | 9 | 8 | ← | 8 | 0 | 8 | 7 | 20526.8868 | 0.0084 |
| 9 | 1 | 9 | 10 | ← | 8 | 0 | 8 | 9 | 20526.8868 | -0.0065 |
| 8 | 2 | 6 | 7 | ← | 7 | 2 | 5 | 6 | 20693.4487 | 0.0015 |
| 8 | 2 | 6 | 9 | ← | 7 | 2 | 5 | 8 | 20693.4487 | -0.0058 |
| 8 | 3 | 5 | 9 | ← | 7 | 3 | 4 | 8 | 20702.1979 | 0.0257 |
| 8 | 3 | 5 | 7 | ← | 7 | 3 | 4 | 6 | 20702.1979 | 0.0220 |
| 6 | 3 | 4 | 7 | ← | 5 | 2 | 4 | 6 | 20951.7440 | 0.0012 |
| 6 | 3 | 4 | 6 | ← | 5 | 2 | 4 | 5 | 20952.0292 | 0.0101 |
| 6 | 3 | 3 | 6 | ← | 5 | 2 | 4 | 5 | 21330.2575 | -0.0098 |
| 9 | 1 | 8 | 8 | ← | 8 | 2 | 7 | 7 | 21357.0577 | 0.0183 |
| 9 | 1 | 8 | 10 | ← | 8 | 2 | 7 | 9 | 21357.0577 | 0.0120 |
| 7 | 3 | 5 | 8 | ← | 6 | 2 | 4 | 7 | 21557.6671 | 0.0206 |
| 7 | 2 | 5 | 8 | ← | 6 | 1 | 5 | 7 | 21559.6729 | 0.0184 |
| 9 | 2 | 8 | 8 | ← | 8 | 2 | 7 | 7 | 21588.0159 | 0.0054 |
| 9 | 2 | 8 | 10 | ← | 8 | 2 | 7 | 9 | 21588.0159 | -0.0021 |
| 9 | 1 | 8 | 9 | ← | 8 | 1 | 7 | 8 | 21783.0798 | 0.0318 |
| 9 | 1 | 8 | 8 | ← | 8 | 1 | 7 | 7 | 21783.0798 | 0.0040 |
| 9 | 1 | 8 | 10 | ← | 8 | 1 | 7 | 9 | 21783.0798 | -0.0053 |
| 9 | 2 | 8 | 9 | ← | 8 | 1 | 7 | 8 | 22014.0544 | 0.0223 |
| 9 | 2 | 8 | 8 | ← | 8 | 1 | 7 | 7 | 22014.0544 | 0.0077 |
| 9 | 2 | 8 | 10 | ← | 8 | 1 | 7 | 9 | 22014.0544 | -0.0030 |
| 6 | 2 | 4 | 6 | ← | 5 | 1 | 5 | 5 | 22330.3354 | 0.0082 |
| 9 | 3 | 7 | 10 | ← | 8 | 3 | 6 | 9 | 22355.4137 | 0.0284 |
| 9 | 3 | 7 | 8 | ← | 8 | 3 | 6 | 7 | 22355.4137 | 0.0281 |
| 7 | 3 | 4 | 8 | ← | 6 | 2 | 4 | 7 | 22408.6097 | 0.0281 |
| 5 | 5 | 0 | 4 | ← | 4 | 4 | 1 | 5 | 22466.1687 | -0.0056 |
| 5 | 5 | 0 | 6 | ← | 4 | 4 | 1 | 5 | 22466.4884 | -0.0078 |
| 9 | 7 | 3 | 9 | ← | 8 | 7 | 2 | 8 | 22488.8197 | -0.0338 |
| 9 | 7 | 3 | 10 | ← | 8 | 7 | 2 | 9 | 22489.3003 | 0.0122 |
| 9 | 7 | 2 | 10 | ← | 8 | 7 | 1 | 9 | 22489.3003 | -0.0107 |
| 6 | 2 | 4 | 7 | ← | 5 | 0 | 5 | 6 | 22499.2071 | 0.0079 |
| 9 | 6 | 3 | 8 | ← | 8 | 6 | 2 | 9 | 22533.8168 | 0.0075 |
| 9 | 5 | 5 | 10 | ← | 8 | 5 | 4 | 9 | 22597.9296 | -0.0281 |
| 9 | 5 | 4 | 10 | ← | 8 | 5 | 3 | 9 | 22623.0726 | -0.0121 |
| 9 | 5 | 4 | 8 | ← | 8 | 5 | 3 | 9 | 22623.0726 | -0.0305 |
| 9 | 4 | 6 | 10 | ← | 8 | 4 | 5 | 9 | 22624.7717 | -0.0189 |
| 9 | 4 | 6 | 8 | ← | 8 | 4 | 5 | 7 | 22624.7717 | -0.0300 |
| 6 | 4 | 3 | 5 | ← | 5 | 3 | 2 | 6 | 22636.4502 | 0.0162 |
| 6 | 4 | 3 | 7 | ← | 5 | 3 | 2 | 6 | 22636.4502 | -0.0114 |
| 7 | 1 | 6 | 7 | ← | 6 | 0 | 6 | 6 | 22647.3543 | 0.0100 |
| 6 | 4 | 2 | 7 | ← | 5 | 3 | 2 | 6 | 22656.7238 | -0.0233 |
| 6 | 4 | 2 | 6 | ← | 5 | 3 | 2 | 5 | 22656.9973 | -0.0002 |
| 10 | 0 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 22722.2461 | 0.0108 |
| 10 | 0 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 22722.2461 | 0.0044 |
| 10 | 0 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 22722.2461 | -0.0078 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 22725.8697 | 0.0087 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 22725.8697 | 0.0025 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 22725.8697 | -0.0097 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 22730.5246 | 0.0099 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 22730.5246 | 0.0040 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 22730.5246 | -0.0082 |
| 10 | 1 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 22734.1531 | 0.0125 |
| 10 | 1 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 22734.1531 | 0.0068 |
| 10 | 1 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 22734.1531 | -0.0054 |
| 6 | 4 | 3 | 5 | ← | 5 | 3 | 3 | 6 | 22771.0834 | -0.0021 |
| 6 | 4 | 2 | 5 | ← | 5 | 3 | 3 | 6 | 22791.3848 | 0.0137 |
| 6 | 4 | 2 | 7 | ← | 5 | 3 | 3 | 6 | 22791.3848 | -0.0139 |
| 6 | 4 | 2 | 6 | ← | 5 | 3 | 3 | 5 | 22791.6521 | -0.0029 |
| 9 | 2 | 7 | 9 | ← | 8 | 2 | 6 | 8 | 23084.2727 | 0.0259 |
| 9 | 2 | 7 | 8 | ← | 8 | 2 | 6 | 7 | 23084.2727 | -0.0044 |
| 9 | 2 | 7 | 10 | ← | 8 | 2 | 6 | 9 | 23084.2727 | -0.0113 |
| 8 | 3 | 6 | 7 | ← | 7 | 2 | 5 | 6 | 23303.6351 | -0.0127 |
| 9 | 3 | 6 | 8 | ← | 8 | 3 | 5 | 7 | 23418.2361 | 0.0004 |
| 9 | 3 | 6 | 10 | ← | 8 | 3 | 5 | 9 | 23418.2361 | -0.0006 |
| 10 | 1 | 9 | 9 | ← | 9 | 2 | 8 | 8 | 23721.2706 | 0.0033 |
| 10 | 1 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 23721.2706 | -0.0030 |
| 7 | 3 | 5 | 7 | ← | 6 | 2 | 5 | 6 | 23772.9471 | -0.0050 |

| J' | $K_{a'}$ | $K_{c'}$ | F' | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 8 | 23839.9511 | 0.0009 |
| 10 | 2 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 23839.9511 | -0.0060 |
| 10 | 1 | 9 | 10 | ← | 9 | 1 | 8 | 9 | 23952.2346 | 0.0225 |
| 10 | 1 | 9 | 9 | ← | 9 | 1 | 8 | 8 | 23952.2346 | -0.0036 |
| 10 | 1 | 9 | 11 | ← | 9 | 1 | 8 | 10 | 23952.2346 | -0.0114 |
| 10 | 2 | 9 | 10 | ← | 9 | 1 | 8 | 9 | 24070.9190 | 0.0182 |
| 10 | 2 | 9 | 9 | ← | 9 | 1 | 8 | 8 | 24070.9190 | -0.0021 |
| 10 | 2 | 9 | 11 | ← | 9 | 1 | 8 | 10 | 24070.9190 | -0.0105 |
| 7 | 3 | 4 | 6 | ← | 6 | 2 | 5 | 5 | 24623.6137 | 0.0209 |
| 7 | 3 | 4 | 7 | ← | 6 | 2 | 5 | 6 | 24623.9269 | 0.0168 |
| 10 | 3 | 8 | 9 | ← | 9 | 3 | 7 | 8 | 24729.4473 | -0.0072 |
| 10 | 3 | 8 | 11 | ← | 9 | 3 | 7 | 10 | 24729.4473 | -0.0091 |
| 8 | 2 | 6 | 9 | ← | 7 | 1 | 6 | 8 | 24827.1876 | 0.0043 |
| 11 | 0 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 24940.4657 | -0.0079 |
| 11 | 0 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 24940.4657 | -0.0132 |
| 11 | 0 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 24940.4657 | -0.0235 |
| 11 | 1 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 24942.0225 | -0.0133 |
| 11 | 1 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 24942.0225 | -0.0186 |
| 11 | 1 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 24942.0225 | -0.0288 |
| 11 | 0 | 11 | 11 | ← | 10 | 0 | 10 | 10 | 24944.0946 | -0.0048 |
| 11 | 0 | 11 | 10 | ← | 10 | 0 | 10 | 9 | 24944.0946 | -0.0099 |
| 11 | 0 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 24944.0946 | -0.0202 |
| 11 | 1 | 11 | 11 | ← | 10 | 0 | 10 | 10 | 24945.6704 | 0.0087 |
| 11 | 1 | 11 | 10 | ← | 10 | 0 | 10 | 9 | 24945.6704 | 0.0037 |
| 11 | 1 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 24945.6704 | -0.0065 |
| 6 | 5 | 2 | 7 | ← | 5 | 4 | 1 | 6 | 24954.7970 | 0.0205 |
| 6 | 5 | 1 | 7 | ← | 5 | 4 | 2 | 6 | 24959.3641 | 0.0247 |
| 9 | 3 | 7 | 8 | ← | 8 | 2 | 6 | 7 | 24965.5884 | 0.0022 |
| 9 | 3 | 7 | 10 | ← | 8 | 2 | 6 | 9 | 24965.5884 | -0.0136 |
| 10 | 2 | 8 | 10 | ← | 9 | 2 | 7 | 9 | 25360.5289 | -0.0216 |
| 7 | 4 | 3 | 6 | ← | 6 | 3 | 4 | 5 | 25393.3663 | 0.0214 |
| 7 | 4 | 3 | 7 | ← | 6 | 3 | 4 | 6 | 25393.6242 | 0.0102 |
| 10 | 4 | 6 | 9 | ← | 9 | 4 | 5 | 8 | 25661.3365 | 0.0064 |
| | | | | | | | | | RMS | 11.2 kHz |

Table S14 Linelist for Conformer VI of isoleucinol. OMC is the difference between the observed and calculated transition.

| J' | $K_{a'}$ | $K_{c'}$ | F' | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 1 | 0 | ← | 0 | 0 | 0 | 1 | 2237.0272 | -0.0009 |
| 1 | 0 | 1 | 2 | ← | 0 | 0 | 0 | 1 | 2237.2951 | 0.0039 |
| 1 | 0 | 1 | 1 | ← | 0 | 0 | 0 | 1 | 2237.4734 | 0.0067 |
| 2 | 1 | 1 | 2 | ← | 2 | 0 | 2 | 2 | 2317.9386 | -0.0184 |
| 2 | 1 | 1 | 3 | ← | 2 | 0 | 2 | 3 | 2318.9434 | 0.0055 |
| 2 | 0 | 2 | 2 | ← | 1 | 1 | 1 | 1 | 2553.5531 | -0.0029 |
| 2 | 0 | 2 | 2 | ← | 1 | 1 | 1 | 2 | 2554.2212 | -0.0010 |
| 2 | 0 | 2 | 1 | ← | 1 | 1 | 1 | 0 | 2554.8041 | -0.0020 |
| 3 | 1 | 2 | 3 | ← | 3 | 0 | 3 | 3 | 2665.4048 | 0.0087 |
| 3 | 1 | 2 | 4 | ← | 3 | 0 | 3 | 4 | 2666.4636 | 0.0060 |
| 3 | 1 | 2 | 2 | ← | 3 | 0 | 3 | 2 | 2666.8344 | 0.0050 |
| 4 | 1 | 3 | 4 | ← | 4 | 0 | 4 | 4 | 3174.7395 | 0.0018 |
| 4 | 1 | 3 | 5 | ← | 4 | 0 | 4 | 5 | 3175.9129 | 0.0005 |
| 4 | 1 | 3 | 3 | ← | 4 | 0 | 4 | 3 | 3176.2176 | 0.0033 |
| 5 | 1 | 4 | 5 | ← | 5 | 0 | 5 | 5 | 3873.8065 | -0.0045 |
| 6 | 2 | 5 | 7 | ← | 6 | 1 | 5 | 7 | 4067.6269 | 0.0019 |
| 6 | 2 | 5 | 6 | ← | 6 | 1 | 5 | 6 | 4068.3400 | 0.0092 |
| 1 | 1 | 1 | 0 | ← | 0 | 0 | 0 | 1 | 4142.1632 | 0.0000 |
| 1 | 1 | 1 | 2 | ← | 0 | 0 | 0 | 1 | 4143.1643 | 0.0017 |
| 1 | 1 | 1 | 1 | ← | 0 | 0 | 0 | 1 | 4143.8328 | 0.0040 |
| 2 | 1 | 2 | 3 | ← | 1 | 1 | 1 | 2 | 4275.5567 | 0.0001 |
| 2 | 1 | 2 | 2 | ← | 1 | 1 | 1 | 1 | 4275.7896 | -0.0026 |
| 2 | 1 | 2 | 1 | ← | 1 | 1 | 1 | 0 | 4276.0562 | 0.0011 |
| 2 | 1 | 2 | 2 | ← | 1 | 1 | 1 | 2 | 4276.4555 | -0.0028 |
| 3 | 0 | 3 | 2 | ← | 2 | 1 | 1 | 1 | 4333.8386 | -0.0070 |
| 3 | 0 | 3 | 4 | ← | 2 | 1 | 1 | 3 | 4334.3786 | -0.0030 |
| 3 | 0 | 3 | 3 | ← | 2 | 1 | 1 | 3 | 4334.7797 | 0.0009 |
| 3 | 0 | 3 | 3 | ← | 2 | 1 | 1 | 2 | 4335.4879 | -0.0046 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 0 | 1 | ← | 0 | 0 | 0 | 1 | 4341.5711 | 0.0062 |
| 1 | 1 | 0 | 2 | ← | 0 | 0 | 0 | 1 | 4342.4100 | 0.0034 |
| 1 | 1 | 0 | 0 | ← | 0 | 0 | 0 | 1 | 4343.6710 | 0.0018 |
| 2 | 0 | 2 | 1 | ← | 1 | 0 | 1 | 1 | 4459.5048 | 0.0020 |
| 2 | 0 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 4459.8332 | 0.0066 |
| 2 | 0 | 2 | 2 | ← | 1 | 0 | 1 | 2 | 4460.1013 | 0.0077 |
| 5 | 2 | 4 | 4 | ← | 5 | 1 | 4 | 4 | 4592.6968 | 0.0012 |
| 5 | 2 | 4 | 6 | ← | 5 | 1 | 4 | 6 | 4592.8348 | -0.0081 |
| 5 | 2 | 4 | 5 | ← | 5 | 1 | 4 | 5 | 4593.5559 | -0.0106 |
| 2 | 1 | 1 | 1 | ← | 1 | 1 | 0 | 0 | 4672.7804 | -0.0029 |
| 2 | 1 | 1 | 2 | ← | 1 | 1 | 0 | 2 | 4672.9367 | 0.0014 |
| 2 | 1 | 1 | 3 | ← | 1 | 1 | 0 | 2 | 4673.6508 | 0.0017 |
| 2 | 1 | 1 | 2 | ← | 1 | 1 | 0 | 1 | 4673.7723 | -0.0045 |
| 2 | 1 | 1 | 1 | ← | 1 | 1 | 0 | 1 | 4674.8829 | -0.0046 |
| 3 | 0 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 4931.2111 | -0.0022 |
| 3 | 0 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 4931.7157 | -0.0023 |
| 3 | 0 | 3 | 2 | ← | 2 | 1 | 2 | 1 | 4932.0885 | 0.0086 |
| 6 | 2 | 4 | 6 | ← | 6 | 1 | 5 | 6 | 5003.3279 | 0.0079 |
| 6 | 2 | 4 | 7 | ← | 6 | 1 | 5 | 7 | 5003.3279 | 0.0017 |
| 6 | 2 | 4 | 5 | ← | 6 | 1 | 5 | 5 | 5003.3279 | 0.0005 |
| 4 | 2 | 3 | 3 | ← | 4 | 1 | 3 | 3 | 5050.8241 | -0.0020 |
| 4 | 2 | 3 | 5 | ← | 4 | 1 | 3 | 5 | 5051.0234 | 0.0137 |
| 4 | 2 | 3 | 4 | ← | 4 | 1 | 3 | 4 | 5051.7211 | -0.0026 |
| 5 | 2 | 3 | 6 | ← | 5 | 1 | 4 | 6 | 5083.0890 | -0.0050 |
| 5 | 2 | 3 | 5 | ← | 5 | 1 | 4 | 5 | 5083.2843 | 0.0040 |
| 4 | 2 | 2 | 5 | ← | 4 | 1 | 3 | 5 | 5267.6025 | 0.0033 |
| 4 | 2 | 2 | 4 | ← | 4 | 1 | 3 | 4 | 5267.9542 | 0.0014 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 2 | 2 | 5428.5718 | -0.0022 |
| 3 | 2 | 2 | 2 | ← | 3 | 1 | 2 | 2 | 5428.5718 | -0.0026 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 2 | 4 | 5428.8050 | -0.0015 |
| 3 | 2 | 2 | 4 | ← | 3 | 1 | 2 | 4 | 5428.8050 | -0.0017 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 2 | 3 | 5429.4704 | -0.0005 |
| 3 | 2 | 2 | 4 | ← | 3 | 1 | 2 | 3 | 5429.4704 | -0.0006 |
| 3 | 2 | 2 | 2 | ← | 3 | 1 | 2 | 3 | 5429.4704 | -0.0009 |
| 3 | 2 | 1 | 2 | ← | 3 | 1 | 2 | 2 | 5502.0682 | -0.0009 |
| 3 | 2 | 1 | 4 | ← | 3 | 1 | 2 | 4 | 5502.2299 | -0.0008 |
| 3 | 2 | 1 | 3 | ← | 3 | 1 | 2 | 3 | 5502.6946 | 0.0017 |
| 2 | 2 | 1 | 1 | ← | 2 | 1 | 1 | 1 | 5717.4399 | -0.0048 |
| 2 | 2 | 1 | 2 | ← | 2 | 1 | 1 | 2 | 5718.2634 | 0.0004 |
| 2 | 2 | 0 | 2 | ← | 2 | 1 | 1 | 1 | 5731.8772 | 0.0048 |
| 2 | 2 | 0 | 1 | ← | 2 | 1 | 1 | 1 | 5732.2886 | 0.0006 |
| 2 | 2 | 0 | 3 | ← | 2 | 1 | 1 | 3 | 5732.5208 | -0.0153 |
| 2 | 2 | 0 | 2 | ← | 2 | 1 | 1 | 2 | 5732.9814 | -0.0015 |
| 2 | 2 | 0 | 3 | ← | 2 | 1 | 1 | 2 | 5733.2422 | -0.0078 |
| 2 | 2 | 0 | 1 | ← | 2 | 1 | 1 | 2 | 5733.4022 | 0.0036 |
| 4 | 0 | 4 | 3 | ← | 3 | 1 | 2 | 2 | 6139.2277 | 0.0024 |
| 4 | 0 | 4 | 5 | ← | 3 | 1 | 2 | 4 | 6139.6027 | 0.0011 |
| 4 | 0 | 4 | 4 | ← | 3 | 1 | 2 | 3 | 6140.8248 | -0.0011 |
| 2 | 1 | 2 | 1 | ← | 1 | 0 | 1 | 1 | 6180.7596 | 0.0079 |
| 2 | 1 | 2 | 1 | ← | 1 | 0 | 1 | 0 | 6181.1959 | 0.0057 |
| 2 | 1 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 6181.4372 | 0.0093 |
| 2 | 1 | 2 | 2 | ← | 1 | 0 | 1 | 1 | 6182.1639 | 0.0095 |
| 2 | 1 | 2 | 2 | ← | 1 | 0 | 1 | 2 | 6182.3413 | 0.0115 |
| 2 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 2 | 6313.9796 | -0.0042 |
| 2 | 2 | 1 | 3 | ← | 2 | 1 | 2 | 2 | 6314.1729 | 0.0012 |
| 2 | 2 | 1 | 1 | ← | 2 | 1 | 2 | 2 | 6314.2665 | -0.0096 |
| 2 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 3 | 6314.8798 | -0.0058 |
| 2 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 1 | 6315.3758 | -0.0107 |
| 2 | 2 | 1 | 1 | ← | 2 | 1 | 2 | 1 | 6315.6694 | -0.0094 |
| 2 | 2 | 0 | 2 | ← | 2 | 1 | 2 | 2 | 6328.7020 | -0.0018 |
| 2 | 2 | 0 | 3 | ← | 2 | 1 | 2 | 3 | 6329.8681 | -0.0045 |
| 2 | 2 | 0 | 1 | ← | 2 | 1 | 2 | 1 | 6330.5164 | -0.0057 |
| 5 | 1 | 4 | 5 | ← | 4 | 2 | 2 | 4 | 6343.9726 | -0.0015 |
| 5 | 1 | 4 | 6 | ← | 4 | 2 | 2 | 5 | 6344.2704 | 0.0063 |
| 3 | 1 | 3 | 2 | ← | 2 | 1 | 2 | 2 | 6403.2397 | 0.0017 |
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 6404.4933 | 0.0007 |
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 6404.6150 | 0.0159 |

| J' | $K_{a'}$ | $K_{c'}$ | F' | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 3 | 6405.5068 | 0.0059 |
| 5 | 1 | 4 | 5 | ← | 4 | 2 | 3 | 4 | 6560.1947 | -0.0085 |
| 5 | 1 | 4 | 6 | ← | 4 | 2 | 3 | 5 | 6560.8478 | -0.0058 |
| 5 | 1 | 4 | 4 | ← | 4 | 2 | 3 | 3 | 6560.9823 | -0.0089 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 3 | 6621.4825 | 0.0009 |
| 3 | 2 | 2 | 4 | ← | 3 | 1 | 3 | 3 | 6621.4825 | 0.0008 |
| 3 | 2 | 2 | 2 | ← | 3 | 1 | 3 | 3 | 6621.4825 | 0.0005 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 4 | 6622.4909 | 0.0012 |
| 3 | 2 | 2 | 4 | ← | 3 | 1 | 3 | 4 | 6622.4909 | 0.0010 |
| 3 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 2 | 6622.8385 | -0.0041 |
| 3 | 2 | 2 | 2 | ← | 3 | 1 | 3 | 2 | 6622.8385 | -0.0045 |
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 2 | 6652.9107 | -0.0025 |
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 6653.3144 | -0.0050 |
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 1 | 6653.3144 | -0.0142 |
| 3 | 0 | 3 | 3 | ← | 2 | 0 | 2 | 2 | 6653.4444 | -0.0050 |
| 3 | 0 | 3 | 3 | ← | 2 | 0 | 2 | 3 | 6653.7097 | -0.0068 |
| 3 | 2 | 1 | 3 | ← | 3 | 1 | 3 | 3 | 6694.7007 | -0.0027 |
| 3 | 2 | 1 | 4 | ← | 3 | 1 | 3 | 4 | 6695.9109 | -0.0029 |
| 3 | 2 | 1 | 2 | ← | 3 | 1 | 3 | 2 | 6696.3415 | 0.0038 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 1 | 6711.7967 | -0.0080 |
| 3 | 2 | 2 | 3 | ← | 2 | 2 | 1 | 3 | 6711.9083 | -0.0005 |
| 3 | 2 | 2 | 4 | ← | 2 | 2 | 1 | 3 | 6711.9083 | -0.0006 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 3 | 6711.9083 | -0.0009 |
| 3 | 2 | 2 | 3 | ← | 2 | 2 | 1 | 2 | 6712.0915 | -0.0051 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 2 | 6712.0915 | -0.0055 |
| 3 | 2 | 1 | 3 | ← | 2 | 2 | 0 | 3 | 6770.3312 | -0.0003 |
| 3 | 2 | 1 | 2 | ← | 2 | 2 | 0 | 1 | 6770.4496 | -0.0065 |
| 3 | 2 | 1 | 3 | ← | 2 | 2 | 0 | 2 | 6770.5947 | -0.0038 |
| 3 | 2 | 1 | 2 | ← | 2 | 2 | 0 | 3 | 6770.5947 | -0.0100 |
| 3 | 2 | 1 | 2 | ← | 2 | 2 | 0 | 2 | 6770.8700 | -0.0017 |
| 2 | 1 | 1 | 2 | ← | 1 | 0 | 1 | 1 | 6777.8814 | 0.0061 |
| 2 | 1 | 1 | 2 | ← | 1 | 0 | 1 | 2 | 6778.0524 | 0.0018 |
| 2 | 1 | 1 | 3 | ← | 1 | 0 | 1 | 2 | 6778.7653 | 0.0008 |
| 2 | 1 | 1 | 1 | ← | 1 | 0 | 1 | 1 | 6778.9892 | 0.0033 |
| 2 | 1 | 1 | 1 | ← | 1 | 0 | 1 | 0 | 6779.4244 | 0.0001 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 3 | 7000.1674 | -0.0074 |
| 3 | 1 | 2 | 2 | ← | 2 | 1 | 1 | 1 | 7000.6647 | -0.0103 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 7000.8391 | 0.0000 |
| 3 | 1 | 2 | 2 | ← | 2 | 1 | 1 | 2 | 7001.7735 | -0.0121 |
| 4 | 2 | 3 | 4 | ← | 4 | 1 | 4 | 4 | 7035.5921 | 0.0015 |
| 4 | 2 | 3 | 5 | ← | 4 | 1 | 4 | 5 | 7036.5758 | -0.0020 |
| 4 | 2 | 3 | 3 | ← | 4 | 1 | 4 | 3 | 7036.8248 | -0.0069 |
| 4 | 2 | 2 | 4 | ← | 4 | 1 | 4 | 4 | 7251.8150 | -0.0046 |
| 4 | 2 | 2 | 5 | ← | 4 | 1 | 4 | 5 | 7253.1659 | -0.0014 |
| 4 | 2 | 2 | 3 | ← | 4 | 1 | 4 | 3 | 7253.5103 | -0.0036 |
| 4 | 0 | 4 | 3 | ← | 3 | 1 | 3 | 3 | 7332.1300 | -0.0027 |
| 4 | 0 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 7332.8333 | -0.0032 |
| 4 | 0 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 7333.2826 | -0.0020 |
| 4 | 0 | 4 | 3 | ← | 3 | 1 | 3 | 2 | 7333.4894 | -0.0044 |
| 4 | 0 | 4 | 4 | ← | 3 | 1 | 3 | 4 | 7333.8500 | 0.0052 |
| 5 | 2 | 4 | 5 | ← | 5 | 1 | 5 | 5 | 7558.1008 | -0.0026 |
| 5 | 2 | 4 | 6 | ← | 5 | 1 | 5 | 6 | 7559.0808 | -0.0062 |
| 5 | 2 | 4 | 4 | ← | 5 | 1 | 5 | 4 | 7559.2815 | -0.0059 |
| 5 | 0 | 5 | 4 | ← | 4 | 1 | 3 | 3 | 7736.4459 | -0.0060 |
| 5 | 0 | 5 | 6 | ← | 4 | 1 | 3 | 5 | 7736.7517 | -0.0090 |
| 5 | 0 | 5 | 5 | ← | 4 | 1 | 3 | 4 | 7738.1108 | -0.0050 |
| 5 | 2 | 3 | 5 | ← | 5 | 1 | 5 | 5 | 8047.8203 | 0.0030 |
| 5 | 2 | 3 | 6 | ← | 5 | 1 | 5 | 6 | 8049.3311 | -0.0069 |
| 3 | 1 | 3 | 2 | ← | 2 | 0 | 2 | 2 | 8125.4829 | 0.0087 |
| 3 | 1 | 3 | 2 | ← | 2 | 0 | 2 | 1 | 8125.8966 | 0.0070 |
| 3 | 1 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 8126.1010 | 0.0070 |
| 3 | 1 | 3 | 3 | ← | 2 | 0 | 2 | 2 | 8126.8422 | 0.0070 |
| 3 | 1 | 3 | 3 | ← | 2 | 0 | 2 | 3 | 8127.1042 | 0.0019 |
| 6 | 2 | 5 | 6 | ← | 6 | 1 | 6 | 6 | 8189.2559 | 0.0227 |
| 4 | 1 | 4 | 3 | ← | 3 | 1 | 3 | 3 | 8522.3460 | 0.0046 |
| 4 | 1 | 4 | 3 | ← | 3 | 1 | 3 | 2 | 8523.6792 | -0.0232 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 8523.6792 | -0.0281 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 4 | 8524.7114 | -0.0042 |
| 6 | 1 | 5 | 5 | ← | 5 | 2 | 3 | 4 | 8799.6846 | 0.0038 |
| 4 | 0 | 4 | 3 | ← | 3 | 0 | 3 | 2 | 8806.0559 | 0.0011 |
| 4 | 0 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 8806.0559 | -0.0032 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 8806.2216 | -0.0005 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 4 | 8806.6335 | 0.0142 |
| 4 | 2 | 3 | 4 | ← | 3 | 2 | 2 | 4 | 8937.7953 | -0.0209 |
| 4 | 3 | 1 | 5 | ← | 3 | 3 | 0 | 4 | 8980.9606 | 0.0118 |
| 4 | 2 | 2 | 3 | ← | 3 | 2 | 1 | 2 | 9080.8710 | -0.0076 |
| 4 | 2 | 2 | 5 | ← | 3 | 2 | 1 | 4 | 9080.8710 | -0.0113 |
| 4 | 2 | 2 | 3 | ← | 3 | 2 | 1 | 3 | 9081.1416 | -0.0103 |
| 6 | 1 | 5 | 6 | ← | 5 | 2 | 4 | 5 | 9289.2729 | -0.0140 |
| 6 | 1 | 5 | 7 | ← | 5 | 2 | 4 | 6 | 9289.9292 | 0.0019 |
| 4 | 1 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 9315.5126 | -0.0014 |
| 3 | 1 | 2 | 3 | ← | 2 | 0 | 2 | 2 | 9318.8391 | -0.0066 |
| 3 | 1 | 2 | 4 | ← | 2 | 0 | 2 | 3 | 9319.7764 | -0.0005 |
| 3 | 1 | 2 | 2 | ← | 2 | 0 | 2 | 1 | 9320.1520 | -0.0060 |
| 5 | 3 | 3 | 4 | ← | 5 | 2 | 3 | 4 | 9661.8111 | 0.0057 |
| 5 | 0 | 5 | 5 | ← | 4 | 1 | 4 | 4 | 9721.9756 | -0.0070 |
| 5 | 0 | 5 | 6 | ← | 4 | 1 | 4 | 5 | 9722.3304 | 0.0014 |
| 5 | 0 | 5 | 5 | ← | 4 | 1 | 4 | 5 | 9723.0584 | -0.0109 |
| 4 | 1 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 9996.4008 | -0.0025 |
| 4 | 1 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 9997.1003 | 0.0073 |
| 4 | 1 | 4 | 4 | ← | 3 | 0 | 3 | 4 | 9997.4964 | 0.0063 |
| 2 | 2 | 1 | 1 | ← | 1 | 1 | 0 | 0 | 10390.2219 | -0.0061 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 0 | 2 | 10391.1944 | -0.0038 |
| 2 | 2 | 1 | 3 | ← | 1 | 1 | 0 | 2 | 10391.3837 | -0.0023 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 0 | 1 | 10392.0354 | -0.0045 |
| 2 | 2 | 1 | 1 | ← | 1 | 1 | 0 | 1 | 10392.3261 | -0.0061 |
| 2 | 2 | 0 | 1 | ← | 1 | 1 | 0 | 0 | 10405.0655 | -0.0057 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 0 | 2 | 10405.9129 | -0.0053 |
| 2 | 2 | 0 | 3 | ← | 1 | 1 | 0 | 2 | 10406.1819 | -0.0033 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 0 | 1 | 10406.7562 | -0.0037 |
| 2 | 2 | 0 | 1 | ← | 1 | 1 | 0 | 1 | 10407.1694 | -0.0060 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 1 | 1 | 10589.7708 | -0.0052 |
| 2 | 2 | 1 | 1 | ← | 1 | 1 | 1 | 1 | 10590.0651 | -0.0032 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 1 | 2 | 10590.4341 | -0.0080 |
| 2 | 2 | 1 | 3 | ← | 1 | 1 | 1 | 2 | 10590.6246 | -0.0054 |
| 2 | 2 | 1 | 1 | ← | 1 | 1 | 1 | 0 | 10591.7309 | -0.0029 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 1 | 1 | 10604.4921 | -0.0039 |
| 2 | 2 | 0 | 1 | ← | 1 | 1 | 1 | 1 | 10604.9074 | -0.0042 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 1 | 2 | 10605.1581 | -0.0040 |
| 2 | 2 | 0 | 3 | ← | 1 | 1 | 1 | 2 | 10605.4261 | -0.0031 |
| 2 | 2 | 0 | 1 | ← | 1 | 1 | 1 | 0 | 10606.5795 | 0.0024 |
| 5 | 1 | 5 | 6 | ← | 4 | 1 | 4 | 5 | 10631.2139 | 0.0266 |
| 5 | 1 | 5 | 4 | ← | 4 | 1 | 4 | 3 | 10631.2139 | -0.0173 |
| 5 | 1 | 5 | 5 | ← | 4 | 1 | 4 | 5 | 10632.3652 | 0.0217 |
| 5 | 0 | 5 | 4 | ← | 4 | 0 | 4 | 3 | 10912.6690 | 0.0029 |
| 5 | 0 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 10912.6690 | -0.0041 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 10912.8527 | -0.0008 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 5 | 10913.4085 | -0.0051 |
| 5 | 2 | 4 | 6 | ← | 4 | 2 | 3 | 5 | 11153.7172 | 0.0206 |
| 5 | 3 | 3 | 4 | ← | 4 | 3 | 2 | 5 | 11230.5063 | -0.0046 |
| 5 | 3 | 3 | 6 | ← | 4 | 3 | 2 | 5 | 11230.5063 | 0.0091 |
| 5 | 2 | 3 | 6 | ← | 4 | 2 | 2 | 5 | 11427.3686 | 0.0104 |
| 5 | 2 | 3 | 4 | ← | 4 | 2 | 2 | 3 | 11427.3686 | 0.0033 |
| 5 | 1 | 4 | 5 | ← | 4 | 1 | 3 | 4 | 11611.9063 | -0.0206 |
| 5 | 1 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 11821.5169 | -0.0147 |
| 5 | 1 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 11822.1361 | 0.0084 |
| 4 | 1 | 3 | 4 | ← | 3 | 0 | 3 | 3 | 11980.9429 | -0.0168 |
| 4 | 1 | 3 | 5 | ← | 3 | 0 | 3 | 4 | 11981.9586 | -0.0129 |
| 4 | 1 | 3 | 3 | ← | 3 | 0 | 3 | 2 | 11982.2480 | -0.0209 |
| 6 | 0 | 6 | 6 | ← | 5 | 1 | 5 | 5 | 12068.3324 | 0.0006 |
| 6 | 0 | 6 | 7 | ← | 5 | 1 | 5 | 6 | 12068.5936 | 0.0244 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 1 | 12429.2462 | -0.0032 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 1 | 3 | 12429.6456 | -0.0002 |
| 3 | 2 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 12429.6456 | -0.0003 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 3 | 12429.6456 | -0.0006 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 12430.3640 | 0.0043 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 2 | 12430.3640 | 0.0039 |
| 3 | 2 | 1 | 2 | ← | 2 | 1 | 1 | 1 | 12502.7429 | -0.0012 |
| 3 | 2 | 1 | 4 | ← | 2 | 1 | 1 | 3 | 12503.0707 | 0.0006 |
| 3 | 2 | 1 | 3 | ← | 2 | 1 | 1 | 2 | 12503.5788 | -0.0027 |
| 6 | 1 | 6 | 7 | ← | 5 | 1 | 5 | 6 | 12726.3989 | -0.0235 |
| 6 | 0 | 6 | 5 | ← | 5 | 0 | 5 | 4 | 12977.4092 | -0.0140 |
| 6 | 0 | 6 | 7 | ← | 5 | 0 | 5 | 6 | 12977.4092 | -0.0183 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 2 | 2 | 13026.0772 | -0.0033 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 2 | 2 | 13026.0772 | -0.0037 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 2 | 3 | 13026.9809 | -0.0013 |
| 3 | 2 | 2 | 4 | ← | 2 | 1 | 2 | 3 | 13026.9809 | -0.0014 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 2 | 3 | 13026.9809 | -0.0017 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 2 | 1 | 13027.4792 | -0.0044 |
| 3 | 2 | 1 | 3 | ← | 2 | 1 | 2 | 2 | 13099.2969 | -0.0055 |
| 3 | 2 | 1 | 4 | ← | 2 | 1 | 2 | 3 | 13100.4023 | -0.0041 |
| 3 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 1 | 13100.9780 | -0.0003 |
| 6 | 2 | 5 | 5 | ← | 5 | 2 | 4 | 6 | 13357.5241 | 0.0120 |
| 6 | 2 | 5 | 5 | ← | 5 | 2 | 4 | 4 | 13357.5241 | -0.0230 |
| 6 | 2 | 5 | 7 | ← | 5 | 2 | 4 | 6 | 13357.5241 | -0.0281 |
| 6 | 1 | 6 | 5 | ← | 5 | 0 | 5 | 4 | 13635.2495 | 0.0241 |
| 6 | 1 | 6 | 7 | ← | 5 | 0 | 5 | 6 | 13635.2495 | -0.0313 |
| 6 | 1 | 6 | 6 | ← | 5 | 0 | 5 | 5 | 13635.7314 | -0.0307 |
| 6 | 2 | 4 | 7 | ← | 5 | 2 | 3 | 6 | 13802.9863 | -0.0160 |
| 6 | 2 | 4 | 5 | ← | 5 | 2 | 3 | 4 | 13802.9863 | -0.0217 |
| 4 | 2 | 3 | 3 | ← | 3 | 1 | 2 | 2 | 14366.2785 | 0.0128 |
| 4 | 2 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 14366.5361 | 0.0123 |
| 4 | 2 | 3 | 4 | ← | 3 | 1 | 2 | 3 | 14367.2905 | 0.0031 |
| 4 | 2 | 2 | 3 | ← | 3 | 1 | 2 | 2 | 14582.9546 | 0.0067 |
| 4 | 2 | 2 | 5 | ← | 3 | 1 | 2 | 4 | 14583.1085 | -0.0047 |
| 4 | 2 | 2 | 4 | ← | 3 | 1 | 2 | 3 | 14583.5116 | -0.0048 |
| 5 | 1 | 4 | 5 | ← | 4 | 0 | 4 | 4 | 14786.6554 | -0.0092 |
| 5 | 1 | 4 | 6 | ← | 4 | 0 | 4 | 5 | 14787.7699 | -0.0058 |
| 5 | 1 | 4 | 4 | ← | 4 | 0 | 4 | 3 | 14788.0436 | 0.0119 |
| 7 | 0 | 7 | 8 | ← | 6 | 0 | 6 | 7 | 15012.9870 | 0.0290 |
| 7 | 2 | 6 | 6 | ← | 6 | 2 | 5 | 5 | 15547.1834 | -0.0089 |
| 7 | 2 | 6 | 8 | ← | 6 | 2 | 5 | 7 | 15547.1834 | -0.0124 |
| 4 | 2 | 3 | 4 | ← | 3 | 1 | 3 | 3 | 15559.3136 | 0.0157 |
| 4 | 2 | 3 | 5 | ← | 3 | 1 | 3 | 4 | 15560.2229 | 0.0161 |
| 4 | 2 | 3 | 3 | ← | 3 | 1 | 3 | 2 | 15560.5399 | 0.0056 |
| 4 | 2 | 2 | 4 | ← | 3 | 1 | 3 | 3 | 15775.5146 | -0.0123 |
| 4 | 2 | 2 | 5 | ← | 3 | 1 | 3 | 4 | 15776.7939 | -0.0024 |
| 4 | 2 | 2 | 3 | ← | 3 | 1 | 3 | 2 | 15777.2009 | -0.0155 |
| 3 | 3 | 1 | 3 | ← | 2 | 2 | 1 | 2 | 16748.0347 | 0.0022 |
| 3 | 3 | 0 | 2 | ← | 2 | 2 | 1 | 1 | 16748.7753 | -0.0168 |
| 8 | 4 | 4 | 9 | ← | 7 | 4 | 3 | 8 | 18007.2948 | 0.0170 |
| 8 | 4 | 4 | 8 | ← | 7 | 4 | 3 | 7 | 18007.2948 | 0.0097 |
| 8 | 4 | 4 | 7 | ← | 7 | 4 | 3 | 8 | 18007.2948 | 0.0078 |
| 5 | 2 | 4 | 5 | ← | 4 | 1 | 4 | 4 | 18189.3813 | 0.0209 |
| 5 | 2 | 4 | 6 | ← | 4 | 1 | 4 | 5 | 18190.2880 | 0.0136 |
| 8 | 1 | 7 | 9 | ← | 7 | 1 | 6 | 8 | 18314.6128 | 0.0221 |
| 8 | 2 | 6 | 7 | ← | 7 | 2 | 5 | 6 | 18576.5496 | 0.0029 |
| 8 | 2 | 6 | 9 | ← | 7 | 2 | 5 | 8 | 18576.5496 | 0.0000 |
| 5 | 2 | 3 | 5 | ← | 4 | 1 | 4 | 4 | 18679.0971 | 0.0231 |
| 5 | 2 | 3 | 6 | ← | 4 | 1 | 4 | 5 | 18680.5383 | 0.0128 |
| 5 | 2 | 3 | 4 | ← | 4 | 1 | 4 | 3 | 18680.8989 | 0.0197 |
| 11 | 2 | 9 | 10 | ← | 10 | 3 | 8 | 10 | 18717.2083 | 0.0276 |
| 11 | 2 | 9 | 10 | ← | 10 | 3 | 8 | 11 | 18717.2083 | -0.0081 |
| 11 | 2 | 9 | 10 | ← | 10 | 3 | 8 | 9 | 18717.2083 | -0.0116 |
| 9 | 0 | 9 | 10 | ← | 8 | 1 | 8 | 9 | 18749.7995 | 0.0074 |
| 9 | 0 | 9 | 8 | ← | 8 | 1 | 8 | 7 | 18749.7995 | -0.0145 |
| 6 | 2 | 4 | 5 | ← | 5 | 1 | 4 | 4 | 18886.0621 | -0.0020 |
| 4 | 3 | 1 | 3 | ← | 3 | 2 | 1 | 2 | 18944.3535 | -0.0297 |
| 9 | 1 | 9 | 10 | ← | 8 | 1 | 8 | 9 | 18944.8201 | 0.0224 |
| 9 | 1 | 9 | 8 | ← | 8 | 1 | 8 | 7 | 18944.8201 | 0.0095 |
| 9 | 1 | 9 | 9 | ← | 8 | 1 | 8 | 8 | 18944.8201 | -0.0329 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | 0 | 9 | 10 | ← | 8 | 0 | 8 | 9 | 19052.0268 | -0.0057 |
| 9 | 0 | 9 | 8 | ← | 8 | 0 | 8 | 7 | 19052.0268 | -0.0110 |
| 7 | 2 | 6 | 8 | ← | 6 | 1 | 5 | 7 | 19614.8109 | -0.0098 |
| 7 | 2 | 6 | 7 | ← | 6 | 1 | 5 | 6 | 19615.6123 | 0.0209 |
| 9 | 2 | 8 | 8 | ← | 8 | 2 | 7 | 7 | 19877.3761 | -0.0117 |
| 9 | 2 | 8 | 10 | ← | 8 | 2 | 7 | 9 | 19877.3761 | -0.0142 |
| 9 | 7 | 3 | 8 | ← | 8 | 7 | 2 | 9 | 20195.3133 | -0.0033 |
| 9 | 7 | 2 | 10 | ← | 8 | 7 | 1 | 9 | 20195.3133 | 0.0169 |
| 9 | 7 | 3 | 10 | ← | 8 | 7 | 2 | 9 | 20195.3133 | 0.0170 |
| 9 | 7 | 2 | 8 | ← | 8 | 7 | 1 | 7 | 20195.3133 | 0.0279 |
| 9 | 6 | 3 | 8 | ← | 8 | 6 | 2 | 7 | 20209.2927 | 0.0221 |
| 9 | 6 | 3 | 10 | ← | 8 | 6 | 2 | 9 | 20209.2927 | 0.0149 |
| 9 | 6 | 4 | 8 | ← | 8 | 6 | 3 | 9 | 20209.2927 | 0.0129 |
| 9 | 6 | 3 | 8 | ← | 8 | 6 | 2 | 9 | 20209.2927 | 0.0019 |
| 9 | 6 | 4 | 9 | ← | 8 | 6 | 3 | 8 | 20209.2927 | -0.0178 |
| 9 | 6 | 3 | 9 | ← | 8 | 6 | 2 | 8 | 20209.2927 | -0.0288 |
| 9 | 5 | 5 | 8 | ← | 8 | 5 | 4 | 9 | 20232.7257 | -0.0018 |
| 9 | 5 | 5 | 9 | ← | 8 | 5 | 4 | 8 | 20232.7257 | -0.0155 |
| 10 | 1 | 9 | 9 | ← | 9 | 2 | 8 | 10 | 20235.6707 | 0.0079 |
| 21 | 4 | 18 | 20 | ← | 21 | 3 | 19 | 20 | 20235.6707 | 0.0166 |
| 10 | 1 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 20235.6707 | -0.0007 |
| 9 | 3 | 7 | 8 | ← | 8 | 3 | 6 | 7 | 20250.3784 | 0.0154 |
| 9 | 3 | 7 | 8 | ← | 8 | 3 | 6 | 9 | 20250.3784 | 0.0150 |
| 9 | 3 | 7 | 10 | ← | 8 | 3 | 6 | 9 | 20250.3784 | 0.0135 |
| 9 | 3 | 7 | 8 | ← | 8 | 3 | 6 | 8 | 20250.3784 | 0.0121 |
| 9 | 3 | 7 | 9 | ← | 8 | 3 | 6 | 9 | 20250.3784 | -0.0004 |
| 9 | 3 | 7 | 9 | ← | 8 | 3 | 6 | 8 | 20250.3784 | -0.0033 |
| 9 | 4 | 6 | 8 | ← | 8 | 4 | 5 | 7 | 20269.2253 | 0.0109 |
| 9 | 4 | 6 | 10 | ← | 8 | 4 | 5 | 9 | 20269.2253 | 0.0097 |
| 9 | 4 | 6 | 9 | ← | 8 | 4 | 5 | 8 | 20269.2253 | 0.0061 |
| 9 | 4 | 6 | 8 | ← | 8 | 4 | 5 | 9 | 20269.2253 | 0.0033 |
| 9 | 4 | 5 | 9 | ← | 8 | 4 | 4 | 8 | 20289.4587 | 0.0178 |
| 9 | 4 | 5 | 8 | ← | 8 | 4 | 4 | 7 | 20289.4587 | 0.0081 |
| 9 | 4 | 5 | 10 | ← | 8 | 4 | 4 | 9 | 20289.4587 | 0.0082 |
| 9 | 4 | 5 | 8 | ← | 8 | 4 | 4 | 9 | 20289.4587 | -0.0009 |
| 9 | 1 | 8 | 8 | ← | 8 | 1 | 7 | 9 | 20460.0194 | 0.0310 |
| 9 | 3 | 6 | 8 | ← | 8 | 3 | 5 | 7 | 20525.4557 | 0.0318 |
| 9 | 3 | 6 | 8 | ← | 8 | 3 | 5 | 9 | 20525.4557 | 0.0049 |
| 10 | 0 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 20877.4453 | 0.0099 |
| 10 | 0 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 20877.4453 | 0.0081 |
| 10 | 0 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 20877.4453 | -0.0057 |
| 7 | 1 | 6 | 7 | ← | 6 | 0 | 6 | 6 | 20899.0844 | 0.0170 |
| 6 | 2 | 5 | 6 | ← | 5 | 1 | 5 | 5 | 20915.7427 | 0.0215 |
| 9 | 2 | 7 | 9 | ← | 8 | 2 | 6 | 8 | 20940.6775 | 0.0179 |
| 9 | 2 | 7 | 8 | ← | 8 | 2 | 6 | 7 | 20940.6775 | 0.0014 |
| 9 | 2 | 7 | 10 | ← | 8 | 2 | 6 | 9 | 20940.6775 | -0.0048 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 21072.4346 | -0.0064 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 21072.4346 | -0.0129 |
| 5 | 3 | 3 | 6 | ← | 4 | 2 | 2 | 5 | 21089.2446 | 0.0205 |
| 5 | 3 | 2 | 6 | ← | 4 | 2 | 2 | 5 | 21108.3463 | 0.0108 |
| 7 | 2 | 5 | 6 | ← | 6 | 1 | 5 | 5 | 21195.5433 | 0.0309 |
| 8 | 2 | 7 | 8 | ← | 7 | 1 | 6 | 7 | 21216.5626 | 0.0264 |
| 5 | 3 | 2 | 6 | ← | 4 | 2 | 3 | 5 | 21324.9092 | -0.0158 |
| 6 | 2 | 4 | 6 | ← | 5 | 1 | 5 | 5 | 21850.7241 | 0.0137 |
| 6 | 2 | 4 | 7 | ← | 5 | 1 | 5 | 6 | 21852.3603 | 0.0198 |
| 6 | 2 | 4 | 5 | ← | 5 | 1 | 5 | 4 | 21852.6775 | 0.0214 |
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 10 | 22016.0955 | 0.0249 |
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 8 | 22016.0955 | -0.0239 |
| 10 | 2 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 22016.0955 | -0.0261 |
| 10 | 6 | 5 | 9 | ← | 9 | 6 | 4 | 10 | 22468.1687 | 0.0313 |
| 10 | 6 | 5 | 10 | ← | 9 | 6 | 4 | 9 | 22468.1687 | 0.0126 |
| 10 | 6 | 4 | 9 | ← | 9 | 6 | 3 | 8 | 22468.1687 | 0.0033 |
| 10 | 3 | 8 | 9 | ← | 9 | 3 | 7 | 10 | 22491.2948 | 0.0192 |
| 10 | 3 | 8 | 9 | ← | 9 | 3 | 7 | 8 | 22491.2948 | 0.0177 |
| 10 | 3 | 8 | 11 | ← | 9 | 3 | 7 | 10 | 22491.2948 | 0.0157 |
| 10 | 3 | 8 | 10 | ← | 9 | 3 | 7 | 9 | 22491.2948 | -0.0060 |
| 10 | 3 | 8 | 10 | ← | 9 | 3 | 7 | 10 | 22491.2948 | -0.0200 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | 5 | 5 | 10 | ← | 9 | 5 | 4 | 10 | 22501.8034 | 0.0236 |
| 10 | 4 | 7 | 10 | ← | 9 | 4 | 6 | 9 | 22544.0723 | 0.0036 |
| 10 | 4 | 7 | 9 | ← | 9 | 4 | 6 | 8 | 22544.0723 | 0.0017 |
| 10 | 4 | 7 | 11 | ← | 9 | 4 | 6 | 10 | 22544.0723 | 0.0012 |
| 10 | 4 | 7 | 9 | ← | 9 | 4 | 6 | 10 | 22544.0723 | -0.0046 |
| 9 | 2 | 8 | 9 | ← | 8 | 1 | 7 | 8 | 22779.2998 | 0.0252 |
| 11 | 1 | 10 | 12 | ← | 10 | 2 | 9 | 11 | 22823.0926 | 0.0123 |
| 11 | 1 | 10 | 10 | ← | 10 | 2 | 9 | 9 | 22823.0926 | -0.0154 |
| 10 | 3 | 7 | 11 | ← | 9 | 3 | 6 | 10 | 22925.3279 | -0.0108 |
| 10 | 3 | 7 | 9 | ← | 9 | 3 | 6 | 8 | 22925.3279 | -0.0175 |
| 11 | 0 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 22974.2117 | 0.0138 |
| 11 | 0 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 22974.2117 | 0.0020 |
| 11 | 0 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 22974.2117 | -0.0034 |
| 4 | 4 | 1 | 5 | ← | 3 | 3 | 0 | 4 | 22989.2415 | 0.0053 |
| 4 | 4 | 0 | 3 | ← | 3 | 3 | 0 | 2 | 22989.2415 | -0.0033 |
| 4 | 4 | 0 | 5 | ← | 3 | 3 | 0 | 4 | 22989.2415 | -0.0213 |
| 11 | 1 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 23050.2179 | 0.0240 |
| 11 | 1 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 23050.2179 | 0.0149 |
| 11 | 1 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 23050.2179 | -0.0221 |
| 11 | 0 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 23097.0905 | 0.0155 |
| 11 | 0 | 11 | 10 | ← | 10 | 0 | 10 | 9 | 23097.0905 | 0.0087 |
| 6 | 3 | 4 | 7 | ← | 5 | 2 | 3 | 6 | 23149.0827 | 0.0274 |
| 6 | 3 | 4 | 5 | ← | 5 | 2 | 3 | 6 | 23149.0827 | 0.0211 |
| 11 | 1 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 23173.0393 | -0.0318 |
| 6 | 3 | 3 | 5 | ← | 5 | 2 | 3 | 4 | 23205.7370 | 0.0246 |
| 6 | 3 | 3 | 7 | ← | 5 | 2 | 3 | 6 | 23205.7370 | -0.0317 |
| 6 | 3 | 3 | 6 | ← | 5 | 2 | 3 | 5 | 23206.0224 | -0.0049 |
| 10 | 2 | 8 | 9 | ← | 9 | 2 | 7 | 8 | 23273.5591 | 0.0042 |
| 10 | 2 | 8 | 11 | ← | 9 | 2 | 7 | 10 | 23273.5591 | -0.0040 |
| 10 | 2 | 8 | 10 | ← | 9 | 2 | 7 | 9 | 23273.5591 | -0.0148 |
| 17 | 4 | 13 | 16 | ← | 16 | 5 | 11 | 15 | 23639.0666 | -0.0130 |
| 6 | 3 | 4 | 6 | ← | 5 | 2 | 4 | 5 | 23639.0666 | -0.0307 |
| 6 | 3 | 4 | 5 | ← | 5 | 2 | 4 | 6 | 23639.2995 | -0.0131 |
| 8 | 2 | 6 | 8 | ← | 7 | 1 | 6 | 7 | 23651.8890 | -0.0080 |
| 8 | 2 | 6 | 9 | ← | 7 | 1 | 6 | 8 | 23652.1809 | 0.0238 |
| 8 | 2 | 6 | 7 | ← | 7 | 1 | 6 | 6 | 23652.1809 | -0.0021 |
| 6 | 3 | 3 | 6 | ← | 5 | 2 | 4 | 5 | 23695.7642 | 0.0231 |
| 6 | 3 | 3 | 7 | ← | 5 | 2 | 4 | 6 | 23696.0463 | 0.0264 |
| 6 | 3 | 3 | 5 | ← | 5 | 2 | 4 | 6 | 23696.0463 | 0.0085 |
| 6 | 3 | 3 | 5 | ← | 5 | 2 | 4 | 4 | 23696.0463 | -0.0265 |
| 7 | 2 | 6 | 7 | ← | 6 | 1 | 6 | 6 | 23736.5103 | 0.0165 |
| 11 | 2 | 10 | 10 | ← | 10 | 2 | 9 | 9 | 24137.2404 | -0.0048 |
| 11 | 2 | 10 | 12 | ← | 10 | 2 | 9 | 11 | 24137.2404 | -0.0068 |
| 8 | 1 | 7 | 8 | ← | 7 | 0 | 7 | 7 | 24200.6825 | 0.0116 |
| 10 | 2 | 9 | 9 | ← | 9 | 1 | 8 | 10 | 24334.7203 | 0.0240 |
| 10 | 2 | 9 | 11 | ← | 9 | 1 | 8 | 10 | 24334.7203 | -0.0270 |
| 11 | 3 | 9 | 10 | ← | 10 | 3 | 8 | 11 | 24719.6393 | -0.0093 |
| 11 | 3 | 9 | 10 | ← | 10 | 3 | 8 | 9 | 24719.6393 | -0.0129 |
| 11 | 3 | 9 | 12 | ← | 10 | 3 | 8 | 11 | 24719.6393 | -0.0151 |
| 11 | 5 | 7 | 10 | ← | 10 | 5 | 6 | 11 | 24773.0597 | -0.0116 |
| 11 | 5 | 6 | 11 | ← | 10 | 5 | 5 | 10 | 24777.5275 | -0.0124 |
| 11 | 5 | 6 | 10 | ← | 10 | 5 | 5 | 9 | 24777.5275 | -0.0131 |
| 11 | 5 | 6 | 12 | ← | 10 | 5 | 5 | 11 | 24777.5275 | -0.0136 |
| 11 | 4 | 8 | 11 | ← | 10 | 4 | 7 | 10 | 24821.5931 | -0.0017 |
| 11 | 4 | 8 | 10 | ← | 10 | 4 | 7 | 9 | 24821.5931 | -0.0063 |
| 11 | 4 | 8 | 12 | ← | 10 | 4 | 7 | 11 | 24821.5931 | -0.0065 |
| 11 | 4 | 8 | 10 | ← | 10 | 4 | 7 | 11 | 24821.5931 | -0.0123 |
| 11 | 4 | 7 | 11 | ← | 10 | 4 | 6 | 10 | 24904.5695 | 0.0122 |
| 11 | 4 | 7 | 12 | ← | 10 | 4 | 6 | 11 | 24904.5695 | -0.0274 |
| 11 | 4 | 7 | 10 | ← | 10 | 4 | 6 | 9 | 24904.5695 | -0.0298 |
| 12 | 0 | 12 | 13 | ← | 11 | 1 | 11 | 12 | 25049.7042 | 0.0042 |
| 12 | 0 | 12 | 11 | ← | 11 | 1 | 11 | 10 | 25049.7042 | -0.0051 |
| 12 | 0 | 12 | 12 | ← | 11 | 1 | 11 | 11 | 25049.7042 | -0.0207 |
| 7 | 3 | 5 | 8 | ← | 6 | 2 | 4 | 7 | 25090.8537 | 0.0162 |
| 7 | 3 | 5 | 6 | ← | 6 | 2 | 4 | 7 | 25090.8537 | 0.0136 |
| 7 | 3 | 5 | 7 | ← | 6 | 2 | 4 | 6 | 25091.2990 | 0.0055 |
| 7 | 3 | 5 | 6 | ← | 6 | 2 | 4 | 6 | 25091.2990 | -0.0151 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | 1 | 12 | 13 | ← | 11 | 1 | 11 | 12 | 25096.0196 | 0.0172 |
| 12 | 1 | 12 | 11 | ← | 11 | 1 | 11 | 10 | 25096.0196 | 0.0092 |
| 12 | 1 | 12 | 12 | ← | 11 | 1 | 11 | 11 | 25096.0196 | -0.0244 |
| 12 | 0 | 12 | 13 | ← | 11 | 0 | 11 | 12 | 25125.7250 | 0.0290 |
| 12 | 0 | 12 | 11 | ← | 11 | 0 | 11 | 10 | 25125.7250 | 0.0222 |
| 12 | 0 | 12 | 12 | ← | 11 | 0 | 11 | 11 | 25125.7250 | -0.0248 |
| 12 | 1 | 12 | 13 | ← | 11 | 0 | 11 | 12 | 25172.0038 | 0.0053 |
| 12 | 1 | 12 | 11 | ← | 11 | 0 | 11 | 10 | 25172.0038 | 0.0000 |
| 5 | 4 | 2 | 5 | ← | 4 | 3 | 1 | 5 | 25227.4444 | -0.0212 |
| 5 | 4 | 1 | 5 | ← | 4 | 3 | 1 | 4 | 25227.8387 | -0.0078 |
| 5 | 4 | 2 | 4 | ← | 4 | 3 | 2 | 4 | 25232.6431 | 0.0313 |
| 5 | 4 | 1 | 5 | ← | 4 | 3 | 2 | 4 | 25232.6431 | 0.0006 |
| 7 | 2 | 5 | 7 | ← | 6 | 1 | 6 | 6 | 25316.3188 | 0.0023 |
| 11 | 2 | 9 | 10 | ← | 10 | 2 | 8 | 9 | 25567.0016 | 0.0158 |
| 11 | 2 | 9 | 12 | ← | 10 | 2 | 8 | 11 | 25567.0016 | 0.0061 |
| | | | | | | | | | RMS | 10.3 kHz |

Table S15 Linelist for Conformer VII of isoleucinol. OMC is the difference between the observed and calculated transition.

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 1 | 1 | ← | 0 | 0 | 0 | 1 | 2422.3281 | 0.0008 |
| 1 | 0 | 1 | 2 | ← | 0 | 0 | 0 | 1 | 2422.4605 | 0.0025 |
| 2 | 0 | 2 | 1 | ← | 1 | 1 | 0 | 0 | 2908.4636 | 0.0060 |
| 1 | 1 | 1 | 0 | ← | 0 | 0 | 0 | 1 | 4089.3455 | 0.0016 |
| 1 | 1 | 1 | 2 | ← | 0 | 0 | 0 | 1 | 4090.4427 | 0.0034 |
| 1 | 1 | 1 | 1 | ← | 0 | 0 | 0 | 1 | 4091.1748 | 0.0052 |
| 1 | 1 | 0 | 1 | ← | 0 | 0 | 0 | 1 | 4332.7790 | 0.0030 |
| 1 | 1 | 0 | 2 | ← | 0 | 0 | 0 | 1 | 4333.3765 | 0.0007 |
| 1 | 1 | 0 | 0 | ← | 0 | 0 | 0 | 1 | 4334.2857 | 0.0103 |
| 2 | 1 | 2 | 1 | ← | 1 | 1 | 1 | 1 | 4601.0499 | 0.0032 |
| 2 | 1 | 2 | 3 | ← | 1 | 1 | 1 | 2 | 4602.1350 | 0.0011 |
| 2 | 1 | 2 | 1 | ← | 1 | 1 | 1 | 0 | 4602.8727 | 0.0002 |
| 2 | 0 | 2 | 1 | ← | 1 | 0 | 1 | 0 | 4820.0845 | 0.0053 |
| 2 | 0 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 4820.2428 | -0.0084 |
| 2 | 0 | 2 | 2 | ← | 1 | 0 | 1 | 1 | 4820.3335 | -0.0052 |
| 2 | 0 | 2 | 1 | ← | 1 | 0 | 1 | 1 | 4820.4062 | 0.0005 |
| 2 | 1 | 1 | 2 | ← | 1 | 1 | 0 | 2 | 5086.8777 | 0.0031 |
| 2 | 1 | 1 | 1 | ← | 1 | 1 | 0 | 0 | 5087.1899 | -0.0023 |
| 2 | 1 | 1 | 2 | ← | 1 | 1 | 0 | 1 | 5087.4793 | 0.0049 |
| 2 | 1 | 1 | 3 | ← | 1 | 1 | 0 | 2 | 5087.6600 | 0.0029 |
| 3 | 0 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 5720.0644 | 0.0015 |
| 3 | 0 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 5720.6100 | -0.0011 |
| 3 | 0 | 3 | 2 | ← | 2 | 1 | 2 | 1 | 5720.9203 | 0.0017 |
| 2 | 1 | 2 | 1 | ← | 1 | 0 | 1 | 0 | 6269.5636 | 0.0012 |
| 2 | 1 | 2 | 1 | ← | 1 | 0 | 1 | 1 | 6269.8865 | -0.0025 |
| 2 | 1 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 6270.1130 | -0.0022 |
| 4 | 0 | 4 | 5 | ← | 3 | 1 | 2 | 4 | 6834.4599 | -0.0068 |
| 4 | 0 | 4 | 4 | ← | 3 | 1 | 2 | 3 | 6835.5602 | 0.0028 |
| 3 | 1 | 3 | 2 | ← | 2 | 1 | 2 | 2 | 6887.6666 | 0.0057 |
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 6888.5383 | 0.0041 |
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 6888.5383 | -0.0126 |
| 3 | 1 | 3 | 2 | ← | 2 | 1 | 2 | 1 | 6888.6660 | 0.0057 |
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 3 | 6889.1917 | -0.0018 |
| 2 | 1 | 1 | 2 | ← | 1 | 0 | 1 | 1 | 6997.9181 | -0.0050 |
| 2 | 1 | 1 | 3 | ← | 1 | 0 | 1 | 2 | 6998.5709 | -0.0040 |
| 2 | 1 | 1 | 1 | ← | 1 | 0 | 1 | 0 | 6998.8208 | 0.0070 |
| 2 | 1 | 1 | 1 | ← | 1 | 0 | 1 | 1 | 6999.1456 | 0.0051 |
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 1 | 7170.3953 | -0.0066 |
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 2 | 7170.4726 | 0.0037 |
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 7170.4726 | -0.0026 |
| 3 | 0 | 3 | 3 | ← | 2 | 0 | 2 | 2 | 7170.6086 | -0.0039 |
| 3 | 2 | 2 | 3 | ← | 2 | 2 | 1 | 2 | 7267.1662 | -0.0059 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 2 | 7267.1662 | -0.0061 |
| 3 | 2 | 2 | 3 | ← | 2 | 2 | 1 | 3 | 7267.3173 | -0.0040 |
| 3 | 2 | 2 | 4 | ← | 2 | 2 | 1 | 3 | 7267.3173 | -0.0040 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 3 | 7267.3173 | -0.0041 |

| J’ | $K_{a'}$ | $K_{c'}$ | F’ | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 1 | 7267.3988 | -0.0055 |
| 3 | 2 | 1 | 3 | ← | 2 | 2 | 0 | 2 | 7363.8575 | -0.0070 |
| 3 | 2 | 1 | 4 | ← | 2 | 2 | 0 | 3 | 7364.1448 | -0.0075 |
| 3 | 2 | 1 | 2 | ← | 2 | 2 | 0 | 3 | 7364.2512 | 0.0131 |
| 3 | 2 | 1 | 2 | ← | 2 | 2 | 0 | 1 | 7364.2512 | -0.0105 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 3 | 7614.3364 | -0.0055 |
| 3 | 1 | 2 | 2 | ← | 2 | 1 | 1 | 1 | 7615.0076 | 0.0019 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 7615.1714 | 0.0157 |
| 3 | 1 | 2 | 2 | ← | 2 | 1 | 1 | 2 | 7616.2170 | -0.0059 |
| 4 | 0 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 8289.1561 | -0.0094 |
| 4 | 0 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 8289.5452 | -0.0028 |
| 4 | 0 | 4 | 3 | ← | 3 | 1 | 3 | 2 | 8289.7149 | 0.0073 |
| 3 | 1 | 3 | 2 | ← | 2 | 0 | 2 | 1 | 8338.1518 | 0.0081 |
| 3 | 1 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 8338.3973 | -0.0009 |
| 3 | 1 | 3 | 3 | ← | 2 | 0 | 2 | 2 | 8339.1023 | 0.0016 |
| 4 | 1 | 4 | 3 | ← | 3 | 1 | 3 | 3 | 9158.5771 | -0.0036 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 9159.4519 | -0.0103 |
| 4 | 1 | 4 | 3 | ← | 3 | 1 | 3 | 2 | 9159.4519 | -0.0189 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 4 | 9160.1159 | -0.0057 |
| 4 | 0 | 4 | 3 | ← | 3 | 0 | 3 | 2 | 9457.4703 | 0.0210 |
| 4 | 0 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 9457.4703 | -0.0006 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 9457.6565 | 0.0027 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 4 | 9670.5628 | 0.0176 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 3 | 9670.5628 | 0.0175 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 2 | 9670.5628 | 0.0177 |
| 4 | 3 | 2 | 5 | ← | 3 | 3 | 1 | 4 | 9734.6098 | 0.0057 |
| 4 | 3 | 2 | 3 | ← | 3 | 3 | 1 | 4 | 9734.6098 | 0.0007 |
| 4 | 3 | 1 | 4 | ← | 3 | 3 | 0 | 3 | 9743.7611 | -0.0080 |
| 4 | 3 | 1 | 5 | ← | 3 | 3 | 0 | 4 | 9743.9729 | 0.0163 |
| 4 | 3 | 1 | 3 | ← | 3 | 3 | 0 | 4 | 9743.9729 | 0.0058 |
| 4 | 2 | 2 | 4 | ← | 3 | 2 | 1 | 3 | 9902.4860 | 0.0035 |
| 4 | 2 | 2 | 5 | ← | 3 | 2 | 1 | 4 | 9902.6801 | -0.0180 |
| 2 | 2 | 1 | 1 | ← | 1 | 1 | 0 | 0 | 10090.8469 | -0.0032 |
| 2 | 2 | 1 | 3 | ← | 1 | 1 | 0 | 2 | 10091.8239 | -0.0088 |
| 2 | 2 | 1 | 1 | ← | 1 | 1 | 0 | 1 | 10092.3344 | -0.0152 |
| 2 | 2 | 1 | 2 | ← | 1 | 1 | 0 | 1 | 10092.5700 | -0.0117 |
| 4 | 1 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 10120.9443 | -0.0014 |
| 4 | 1 | 3 | 4 | ← | 3 | 1 | 2 | 3 | 10120.9443 | -0.0254 |
| 4 | 1 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 10327.3425 | -0.0009 |
| 2 | 2 | 0 | 2 | ← | 1 | 1 | 1 | 1 | 10358.6936 | -0.0102 |
| 2 | 2 | 0 | 3 | ← | 1 | 1 | 1 | 2 | 10359.3861 | -0.0050 |
| 2 | 2 | 0 | 1 | ← | 1 | 1 | 1 | 0 | 10360.4722 | 0.0093 |
| 5 | 0 | 5 | 6 | ← | 4 | 1 | 4 | 5 | 10811.6419 | 0.0216 |
| 5 | 0 | 5 | 4 | ← | 4 | 0 | 4 | 3 | 11681.4915 | 0.0213 |
| 5 | 0 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 11681.4915 | -0.0012 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 11681.6761 | 0.0002 |
| 5 | 2 | 4 | 4 | ← | 4 | 2 | 3 | 3 | 12057.4993 | 0.0161 |
| 5 | 2 | 4 | 6 | ← | 4 | 2 | 3 | 5 | 12057.4993 | 0.0127 |
| 5 | 2 | 4 | 4 | ← | 4 | 2 | 3 | 5 | 12057.4993 | 0.0069 |
| 5 | 2 | 4 | 5 | ← | 4 | 2 | 3 | 4 | 12057.4993 | 0.0052 |
| 5 | 3 | 2 | 5 | ← | 4 | 3 | 1 | 4 | 12213.6076 | -0.0095 |
| 5 | 3 | 2 | 6 | ← | 4 | 3 | 1 | 5 | 12213.7486 | 0.0006 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 1 | 12271.0570 | -0.0053 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 1 | 3 | 12271.4953 | -0.0016 |
| 3 | 2 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 12271.4953 | -0.0016 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 3 | 12271.4953 | -0.0018 |
| 3 | 2 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 12272.2632 | -0.0163 |
| 3 | 2 | 2 | 2 | ← | 2 | 1 | 1 | 2 | 12272.2632 | -0.0164 |
| 5 | 1 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 12283.1546 | 0.0022 |
| 5 | 2 | 3 | 5 | ← | 4 | 2 | 2 | 4 | 12487.2784 | 0.0024 |
| 5 | 2 | 3 | 6 | ← | 4 | 2 | 2 | 5 | 12487.4443 | -0.0085 |
| 5 | 2 | 3 | 4 | ← | 4 | 2 | 2 | 3 | 12487.4443 | -0.0200 |
| 5 | 1 | 4 | 5 | ← | 4 | 1 | 3 | 4 | 12594.1546 | -0.0181 |
| 5 | 1 | 4 | 4 | ← | 4 | 1 | 3 | 4 | 12595.0269 | -0.0212 |
| 3 | 2 | 1 | 3 | ← | 2 | 1 | 2 | 2 | 13120.5202 | -0.0021 |
| 3 | 2 | 1 | 4 | ← | 2 | 1 | 2 | 3 | 13121.3965 | -0.0131 |
| 3 | 2 | 1 | 2 | ← | 2 | 1 | 2 | 1 | 13121.8316 | -0.0206 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | 0 | 6 | 5 | ← | 5 | 0 | 5 | 4 | 13860.4673 | 0.0126 |
| 6 | 0 | 6 | 7 | ← | 5 | 0 | 5 | 6 | 13860.4673 | 0.0012 |
| 6 | 0 | 6 | 6 | ← | 5 | 0 | 5 | 5 | 13860.6541 | 0.0251 |
| 4 | 2 | 3 | 3 | ← | 3 | 1 | 2 | 2 | 14326.5851 | -0.0166 |
| 4 | 2 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 14326.8804 | 0.0029 |
| 4 | 2 | 3 | 4 | ← | 3 | 1 | 2 | 3 | 14327.6388 | -0.0170 |
| 6 | 2 | 5 | 6 | ← | 5 | 2 | 4 | 6 | 14424.5842 | 0.0109 |
| 6 | 2 | 5 | 5 | ← | 5 | 2 | 4 | 5 | 14424.5842 | -0.0130 |
| 6 | 3 | 4 | 7 | ← | 5 | 3 | 3 | 6 | 14630.3677 | 0.0073 |
| 6 | 3 | 4 | 5 | ← | 5 | 3 | 3 | 4 | 14630.3677 | 0.0014 |
| 7 | 0 | 7 | 8 | ← | 6 | 0 | 6 | 7 | 16018.7681 | -0.0196 |
| 8 | 1 | 8 | 9 | ← | 7 | 1 | 7 | 8 | 18076.3802 | 0.0167 |
| 8 | 1 | 8 | 7 | ← | 7 | 1 | 7 | 6 | 18076.3802 | 0.0075 |
| 6 | 2 | 5 | 5 | ← | 5 | 1 | 4 | 5 | 18094.6205 | 0.0158 |
| 6 | 2 | 5 | 5 | ← | 5 | 1 | 4 | 5 | 18094.6205 | 0.0158 |
| 8 | 0 | 8 | 9 | ← | 7 | 0 | 7 | 8 | 18174.1659 | -0.0132 |
| 8 | 0 | 8 | 7 | ← | 7 | 0 | 7 | 6 | 18174.1659 | -0.0144 |
| 8 | 2 | 7 | 9 | ← | 7 | 2 | 6 | 8 | 19088.2382 | 0.0064 |
| 6 | 1 | 5 | 6 | ← | 5 | 0 | 5 | 5 | 19219.2769 | 0.0175 |
| 5 | 2 | 3 | 6 | ← | 4 | 1 | 4 | 5 | 19463.6300 | 0.0239 |
| 5 | 2 | 3 | 4 | ← | 4 | 1 | 4 | 3 | 19463.9304 | 0.0141 |
| 8 | 3 | 6 | 8 | ← | 7 | 3 | 5 | 7 | 19513.6898 | 0.0213 |
| 8 | 3 | 6 | 7 | ← | 7 | 3 | 5 | 6 | 19513.6898 | 0.0080 |
| 8 | 3 | 6 | 9 | ← | 7 | 3 | 5 | 8 | 19513.6898 | 0.0061 |
| 8 | 3 | 6 | 7 | ← | 7 | 3 | 5 | 8 | 19513.6898 | -0.0223 |
| 8 | 4 | 5 | 9 | ← | 7 | 4 | 4 | 8 | 19541.6394 | -0.0075 |
| 8 | 4 | 5 | 7 | ← | 7 | 4 | 4 | 6 | 19541.6394 | -0.0120 |
| 8 | 4 | 5 | 7 | ← | 7 | 4 | 4 | 8 | 19541.6394 | -0.0334 |
| 6 | 2 | 4 | 6 | ← | 5 | 1 | 4 | 5 | 19548.5446 | 0.0325 |
| 6 | 2 | 4 | 5 | ← | 5 | 1 | 4 | 4 | 19548.5446 | 0.0106 |
| 6 | 2 | 4 | 7 | ← | 5 | 1 | 4 | 6 | 19548.5446 | -0.0077 |
| 8 | 4 | 4 | 9 | ← | 7 | 4 | 3 | 8 | 19567.7861 | 0.0184 |
| 8 | 4 | 4 | 7 | ← | 7 | 4 | 3 | 6 | 19567.7861 | 0.0121 |
| 8 | 4 | 4 | 7 | ← | 7 | 4 | 3 | 8 | 19567.7861 | -0.0109 |
| 8 | 1 | 7 | 7 | ← | 7 | 1 | 6 | 8 | 19683.6867 | 0.0055 |
| 7 | 2 | 6 | 6 | ← | 6 | 1 | 5 | 7 | 19841.4391 | 0.0065 |
| 7 | 2 | 6 | 8 | ← | 6 | 1 | 5 | 7 | 19841.4391 | -0.0005 |
| 7 | 2 | 6 | 7 | ← | 6 | 1 | 5 | 6 | 19842.1204 | 0.0014 |
| 8 | 3 | 5 | 9 | ← | 7 | 3 | 4 | 8 | 19847.1486 | -0.0075 |
| 8 | 3 | 5 | 7 | ← | 7 | 3 | 4 | 6 | 19847.1486 | -0.0164 |
| 9 | 1 | 8 | 8 | ← | 8 | 2 | 7 | 7 | 20050.2989 | 0.0138 |
| 9 | 0 | 9 | 10 | ← | 8 | 1 | 8 | 9 | 20192.4846 | 0.0131 |
| 9 | 0 | 9 | 8 | ← | 8 | 1 | 8 | 7 | 20192.4846 | 0.0017 |
| 9 | 0 | 9 | 9 | ← | 8 | 1 | 8 | 8 | 20192.4846 | -0.0013 |
| 8 | 2 | 6 | 8 | ← | 7 | 2 | 5 | 7 | 20267.1460 | 0.0310 |
| 8 | 2 | 6 | 7 | ← | 7 | 2 | 5 | 6 | 20267.1460 | 0.0154 |
| 8 | 2 | 6 | 9 | ← | 7 | 2 | 5 | 8 | 20267.1460 | 0.0035 |
| 9 | 1 | 9 | 10 | ← | 8 | 1 | 8 | 9 | 20274.0135 | 0.0175 |
| 9 | 1 | 9 | 8 | ← | 8 | 1 | 8 | 7 | 20274.0135 | 0.0099 |
| 9 | 1 | 9 | 9 | ← | 8 | 1 | 8 | 8 | 20274.0135 | -0.0298 |
| 9 | 0 | 9 | 10 | ← | 8 | 0 | 8 | 9 | 20334.3124 | -0.0005 |
| 9 | 0 | 9 | 8 | ← | 8 | 0 | 8 | 7 | 20334.3124 | -0.0041 |
| 9 | 1 | 9 | 8 | ← | 8 | 0 | 8 | 7 | 20415.8461 | 0.0088 |
| 9 | 1 | 9 | 10 | ← | 8 | 0 | 8 | 9 | 20415.8461 | 0.0087 |
| 5 | 3 | 3 | 6 | ← | 4 | 2 | 3 | 5 | 21207.6098 | 0.0076 |
| 5 | 3 | 3 | 4 | ← | 4 | 2 | 3 | 3 | 21207.6098 | -0.0070 |
| 9 | 2 | 8 | 8 | ← | 8 | 2 | 7 | 9 | 21382.1414 | 0.0122 |
| 9 | 2 | 8 | 8 | ← | 8 | 2 | 7 | 7 | 21382.1414 | -0.0011 |
| 9 | 2 | 8 | 10 | ← | 8 | 2 | 7 | 9 | 21382.1414 | -0.0068 |
| 8 | 2 | 7 | 8 | ← | 7 | 1 | 6 | 7 | 21542.2909 | 0.0163 |
| 6 | 2 | 5 | 6 | ← | 5 | 1 | 5 | 5 | 21691.0311 | -0.0101 |
| 9 | 1 | 8 | 8 | ← | 8 | 1 | 7 | 9 | 21908.3226 | 0.0197 |
| 9 | 3 | 7 | 8 | ← | 8 | 3 | 6 | 7 | 21936.3098 | 0.0131 |
| 9 | 3 | 7 | 10 | ← | 8 | 3 | 6 | 9 | 21936.3098 | 0.0098 |
| 9 | 3 | 7 | 9 | ← | 8 | 3 | 6 | 8 | 21936.3098 | 0.0081 |
| 9 | 5 | 5 | 9 | ← | 8 | 5 | 4 | 8 | 21963.1245 | 0.0296 |
| 9 | 5 | 5 | 10 | ← | 8 | 5 | 4 | 9 | 21963.1245 | -0.0288 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | 5 | 4 | 10 | ← | 8 | 5 | 3 | 9 | 21965.9048 | 0.0048 |
| 9 | 5 | 4 | 8 | ← | 8 | 5 | 3 | 7 | 21965.9048 | -0.0004 |
| 9 | 4 | 6 | 10 | ← | 8 | 4 | 5 | 9 | 22013.2128 | 0.0187 |
| 9 | 4 | 6 | 8 | ← | 8 | 4 | 5 | 7 | 22013.2128 | 0.0164 |
| 9 | 4 | 5 | 10 | ← | 8 | 4 | 4 | 9 | 22073.9826 | 0.0190 |
| 9 | 4 | 5 | 8 | ← | 8 | 4 | 4 | 7 | 22073.9826 | 0.0137 |
| 9 | 4 | 5 | 8 | ← | 8 | 4 | 4 | 9 | 22073.9826 | -0.0156 |
| 4 | 4 | 1 | 3 | ← | 3 | 3 | 1 | 2 | 22220.6300 | 0.0302 |
| 4 | 4 | 1 | 4 | ← | 3 | 3 | 1 | 3 | 22220.6300 | 0.0046 |
| 7 | 2 | 5 | 8 | ← | 6 | 1 | 5 | 7 | 22224.5062 | 0.0021 |
| 7 | 2 | 5 | 6 | ← | 6 | 1 | 5 | 5 | 22224.5062 | -0.0134 |
| 10 | 0 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 22418.9550 | 0.0126 |
| 10 | 0 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 22418.9550 | 0.0042 |
| 10 | 0 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 22418.9550 | -0.0125 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 22464.7735 | 0.0134 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 22464.7735 | 0.0068 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 22464.7735 | -0.0290 |
| 9 | 3 | 6 | 10 | ← | 8 | 3 | 5 | 9 | 22483.5317 | 0.0053 |
| 9 | 3 | 6 | 8 | ← | 8 | 3 | 5 | 7 | 22483.5317 | -0.0014 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 22500.4800 | 0.0131 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 22500.4800 | 0.0084 |
| 10 | 1 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 22546.2632 | -0.0213 |
| 10 | 1 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 22546.2632 | -0.0241 |
| 10 | 1 | 9 | 9 | ← | 9 | 2 | 8 | 10 | 22745.2517 | -0.0322 |
| 10 | 1 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 22745.2517 | -0.0323 |
| 9 | 2 | 7 | 8 | ← | 8 | 2 | 6 | 7 | 22788.5468 | 0.0127 |
| 9 | 2 | 7 | 10 | ← | 8 | 2 | 6 | 9 | 22788.5468 | -0.0016 |
| 9 | 2 | 7 | 9 | ← | 8 | 2 | 6 | 8 | 22788.5468 | -0.0182 |
| 9 | 2 | 8 | 8 | ← | 8 | 1 | 7 | 7 | 23240.1471 | 0.0296 |
| 9 | 2 | 8 | 9 | ← | 8 | 1 | 7 | 8 | 23240.6951 | 0.0049 |
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 10 | 23651.3620 | 0.0067 |
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 8 | 23651.3620 | -0.0124 |
| 10 | 2 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 23651.3620 | -0.0170 |
| 10 | 3 | 8 | 9 | ← | 9 | 3 | 7 | 8 | 24338.7408 | -0.0266 |
| 10 | 3 | 8 | 11 | ← | 9 | 3 | 7 | 10 | 24338.7408 | -0.0308 |
| 10 | 5 | 6 | 10 | ← | 9 | 5 | 5 | 9 | 24434.7018 | 0.0164 |
| 10 | 5 | 5 | 11 | ← | 9 | 5 | 4 | 10 | 24442.3037 | 0.0119 |
| 10 | 5 | 5 | 9 | ← | 9 | 5 | 4 | 8 | 24442.3037 | 0.0084 |
| 10 | 5 | 5 | 9 | ← | 9 | 5 | 4 | 10 | 24442.3037 | -0.0096 |
| 10 | 4 | 7 | 11 | ← | 9 | 4 | 6 | 10 | 24487.0254 | -0.0122 |
| 10 | 4 | 7 | 9 | ← | 9 | 4 | 6 | 8 | 24487.0254 | -0.0130 |
| 11 | 0 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 24625.6761 | 0.0085 |
| 11 | 0 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 24625.6761 | 0.0018 |
| 11 | 0 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 24625.6761 | -0.0201 |
| 11 | 1 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 24650.9642 | -0.0035 |
| 11 | 1 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 24650.9642 | -0.0093 |
| 11 | 0 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 24671.4753 | -0.0098 |
| 11 | 0 | 11 | 10 | ← | 10 | 0 | 10 | 9 | 24671.4753 | -0.0147 |
| 11 | 1 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 24696.7962 | 0.0108 |
| 11 | 1 | 11 | 10 | ← | 10 | 0 | 10 | 9 | 24696.7962 | 0.0067 |
| 7 | 2 | 6 | 6 | ← | 6 | 1 | 6 | 5 | 24812.0140 | 0.0191 |
| 10 | 2 | 9 | 11 | ← | 9 | 1 | 8 | 10 | 24983.2729 | -0.0016 |
| 10 | 2 | 8 | 10 | ← | 9 | 2 | 7 | 9 | 25248.7632 | -0.0100 |
| | | | | | | | | | RMS | 10.5 kHz |

# S7 Linelist for the isotopologues of Conformers I, II and III of isoleucinol

## S7.1 Isotopologues of Conformers I

Table S16 Linelist for $^{13}$C1 isotopologue of Conformer I of isoleucinol. OMC is the difference between the observed and calculated transition.

| *J'* | $K_{a'}$ | $K_{c'}$ | *F'* | | *J* | $K_a$ | $K_c$ | *F* | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 0 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 3851.2428 | 0.0015 |
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 5513.9318 | -0.0037 |
| 3 | 1 | 3 | 2 | ← | 2 | 1 | 2 | 1 | 5513.9318 | -0.0103 |
| 3 | 0 | 3 | 3 | ← | 2 | 0 | 2 | 2 | 5754.9426 | 0.0158 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6055.0976 | 0.0080 |
| 3 | 1 | 2 | 2 | ← | 2 | 1 | 1 | 3 | 6055.4839 | -0.0030 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 7342.0190 | -0.0063 |
| 4 | 1 | 4 | 3 | ← | 3 | 1 | 3 | 2 | 7342.1348 | -0.0045 |
| 4 | 1 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 7342.1957 | 0.0079 |
| 4 | 0 | 4 | 3 | ← | 3 | 0 | 3 | 2 | 7633.2041 | 0.0039 |
| 4 | 0 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 7633.3291 | 0.0043 |
| 4 | 2 | 2 | 4 | ← | 3 | 2 | 1 | 3 | 7799.1380 | 0.0014 |
| 4 | 2 | 2 | 5 | ← | 3 | 2 | 1 | 4 | 7799.7196 | -0.0052 |
| 4 | 2 | 2 | 3 | ← | 3 | 2 | 1 | 2 | 7799.8784 | 0.0041 |
| 4 | 2 | 2 | 3 | ← | 3 | 2 | 1 | 4 | 7799.8784 | -0.0029 |
| 4 | 1 | 3 | 4 | ← | 3 | 1 | 2 | 3 | 8062.3087 | -0.0032 |
| 4 | 1 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 8062.4696 | -0.0078 |
| 5 | 1 | 5 | 6 | ← | 4 | 1 | 4 | 5 | 9162.9728 | 0.0032 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 9480.1857 | -0.0256 |
| 5 | 1 | 4 | 6 | ← | 4 | 1 | 3 | 5 | 10059.7498 | 0.0049 |
| 6 | 0 | 6 | 6 | ← | 5 | 0 | 5 | 5 | 11293.0894 | -0.0128 |
| 6 | 2 | 5 | 5 | ← | 5 | 2 | 4 | 4 | 11540.3734 | -0.0013 |
| 6 | 2 | 5 | 7 | ← | 5 | 2 | 4 | 6 | 11540.3734 | -0.0019 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 18137.5072 | -0.0010 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 18137.5072 | -0.0052 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 18137.5072 | -0.0151 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 18303.1093 | 0.0080 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 18303.1093 | -0.0080 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 18303.1093 | -0.0133 |
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 8 | 19082.1650 | 0.0107 |
| 10 | 2 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 19082.1650 | -0.0001 |
| 10 | 1 | 9 | 11 | ← | 9 | 1 | 8 | 10 | 19749.0161 | 0.0038 |
| 10 | 1 | 9 | 10 | ← | 9 | 1 | 8 | 9 | 19749.0161 | 0.0036 |
| 11 | 1 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 19909.2300 | -0.0060 |
| 11 | 1 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 19909.2300 | -0.0108 |
| 11 | 1 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 19909.2300 | -0.0178 |
| 11 | 0 | 11 | 10 | ← | 10 | 0 | 10 | 9 | 20034.0065 | 0.0149 |
| 11 | 0 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 20034.0065 | 0.0019 |
| 11 | 0 | 11 | 11 | ← | 10 | 0 | 10 | 10 | 20034.0065 | -0.0016 |
| 10 | 2 | 8 | 10 | ← | 9 | 2 | 7 | 9 | 20067.3006 | 0.0255 |
| 10 | 2 | 8 | 9 | ← | 9 | 2 | 7 | 8 | 20067.3006 | -0.0099 |
| 10 | 2 | 8 | 11 | ← | 9 | 2 | 7 | 10 | 20067.3006 | -0.0210 |
| 11 | 2 | 10 | 10 | ← | 10 | 2 | 9 | 9 | 20938.0647 | 0.0245 |
| 11 | 2 | 10 | 12 | ← | 10 | 2 | 9 | 11 | 20938.0647 | 0.0147 |
| 11 | 1 | 10 | 10 | ← | 10 | 1 | 9 | 9 | 21594.4590 | 0.0006 |
| 11 | 1 | 10 | 12 | ← | 10 | 1 | 9 | 11 | 21594.4590 | -0.0136 |
| 11 | 1 | 10 | 11 | ← | 10 | 1 | 9 | 10 | 21594.4590 | -0.0189 |
| 12 | 1 | 12 | 12 | ← | 11 | 1 | 11 | 11 | 21675.4320 | 0.0022 |
| 12 | 1 | 12 | 13 | ← | 11 | 1 | 11 | 12 | 21675.4320 | -0.0027 |
| 12 | 0 | 12 | 11 | ← | 11 | 0 | 11 | 10 | 21766.5789 | 0.0082 |
| 12 | 0 | 12 | 13 | ← | 11 | 0 | 11 | 12 | 21766.5789 | -0.0024 |
| 12 | 0 | 12 | 12 | ← | 11 | 0 | 11 | 11 | 21766.5789 | -0.0046 |
| 11 | 2 | 9 | 11 | ← | 10 | 2 | 8 | 10 | 22111.2264 | 0.0136 |
| 11 | 2 | 9 | 10 | ← | 10 | 2 | 8 | 9 | 22111.2264 | -0.0089 |
| 11 | 2 | 9 | 12 | ← | 10 | 2 | 8 | 11 | 22111.2264 | -0.0192 |
| 12 | 2 | 11 | 11 | ← | 11 | 2 | 10 | 10 | 22780.9742 | 0.0003 |
| 12 | 2 | 11 | 13 | ← | 11 | 2 | 10 | 12 | 22780.9742 | -0.0084 |
| 13 | 0 | 13 | 12 | ← | 12 | 0 | 12 | 11 | 23502.1787 | 0.0230 |
| 13 | 0 | 13 | 14 | ← | 12 | 0 | 12 | 13 | 23502.1787 | 0.0141 |
| 13 | 0 | 13 | 13 | ← | 12 | 0 | 12 | 12 | 23502.1787 | 0.0130 |

| | |
|---|---|
| RMS | 8.7 kHz |

Table S17 Linelist for $^{13}$C2 isotopologue of Conformer I of isoleucinol. OMC is the difference between the observed and calculated transition.

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 0 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 3873.3136 | 0.0063 |
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 5545.0709 | -0.0020 |
| 3 | 1 | 3 | 2 | ← | 2 | 1 | 2 | 1 | 5545.0709 | -0.0086 |
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 1 | 5787.5088 | -0.0025 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 6089.9833 | 0.0055 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6090.3669 | 0.0122 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 7383.4109 | -0.0058 |
| 4 | 0 | 4 | 3 | ← | 3 | 0 | 3 | 2 | 7676.4212 | -0.0042 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 7676.5461 | 0.0127 |
| 4 | 0 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 7676.5461 | -0.0038 |
| 4 | 0 | 4 | 3 | ← | 3 | 0 | 3 | 3 | 7678.2874 | -0.0095 |
| 4 | 2 | 3 | 4 | ← | 3 | 2 | 2 | 3 | 7756.8590 | -0.0103 |
| 4 | 2 | 3 | 4 | ← | 3 | 2 | 2 | 4 | 7756.8590 | -0.0105 |
| 4 | 2 | 3 | 5 | ← | 3 | 2 | 2 | 4 | 7757.4369 | -0.0054 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 2 | 7757.5850 | -0.0044 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 3 | 7757.5850 | -0.0048 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 4 | 7757.5850 | -0.0050 |
| 4 | 2 | 2 | 5 | ← | 3 | 2 | 1 | 4 | 7845.1429 | 0.0024 |
| 4 | 1 | 3 | 4 | ← | 3 | 1 | 2 | 3 | 8109.1674 | -0.0158 |
| 5 | 1 | 5 | 6 | ← | 4 | 1 | 4 | 5 | 9214.5449 | 0.0230 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 9533.4507 | -0.0207 |
| 5 | 0 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 9533.4507 | -0.0246 |
| 5 | 1 | 4 | 6 | ← | 4 | 1 | 3 | 5 | 10118.0832 | 0.0042 |
| 6 | 1 | 6 | 6 | ← | 5 | 1 | 5 | 5 | 11036.8383 | -0.0150 |
| 6 | 2 | 5 | 5 | ← | 5 | 2 | 4 | 4 | 11606.4133 | 0.0147 |
| 6 | 2 | 5 | 7 | ← | 5 | 2 | 4 | 6 | 11606.4133 | 0.0142 |
| 9 | 2 | 7 | 8 | ← | 8 | 2 | 6 | 7 | 18113.8485 | 0.0220 |
| 9 | 2 | 7 | 10 | ← | 8 | 2 | 6 | 9 | 18113.8485 | 0.0103 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 18238.5084 | 0.0051 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 18238.5084 | 0.0009 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 18238.5084 | -0.0089 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 18403.6625 | 0.0167 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 18403.6625 | 0.0005 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 18403.6625 | -0.0046 |
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 8 | 19190.2490 | 0.0286 |
| 10 | 2 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 19190.2490 | 0.0177 |
| 10 | 1 | 9 | 9 | ← | 9 | 1 | 8 | 8 | 19860.3086 | 0.0148 |
| 10 | 1 | 9 | 11 | ← | 9 | 1 | 8 | 10 | 19860.3086 | -0.0018 |
| 10 | 1 | 9 | 10 | ← | 9 | 1 | 8 | 9 | 19860.3086 | -0.0021 |
| 11 | 1 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 20019.9391 | 0.0038 |
| 11 | 1 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 20019.9391 | -0.0009 |
| 11 | 1 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 20019.9391 | -0.0078 |
| 11 | 0 | 11 | 10 | ← | 10 | 0 | 10 | 9 | 20144.1315 | 0.0073 |
| 11 | 0 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 20144.1315 | -0.0056 |
| 11 | 0 | 11 | 11 | ← | 10 | 0 | 10 | 10 | 20144.1315 | -0.0091 |
| 10 | 2 | 8 | 10 | ← | 9 | 2 | 7 | 9 | 20185.4560 | 0.0213 |
| 10 | 2 | 8 | 9 | ← | 9 | 2 | 7 | 8 | 20185.4560 | -0.0139 |
| 10 | 2 | 8 | 11 | ← | 9 | 2 | 7 | 10 | 20185.4560 | -0.0251 |
| 11 | 2 | 10 | 11 | ← | 10 | 2 | 9 | 10 | 21056.2624 | 0.0198 |
| 11 | 2 | 10 | 10 | ← | 10 | 2 | 9 | 9 | 21056.2624 | 0.0040 |
| 11 | 2 | 10 | 12 | ← | 10 | 2 | 9 | 11 | 21056.2624 | -0.0057 |
| 11 | 1 | 10 | 10 | ← | 10 | 1 | 9 | 9 | 21715.0870 | -0.0029 |
| 11 | 1 | 10 | 12 | ← | 10 | 1 | 9 | 11 | 21715.0870 | -0.0172 |
| 11 | 1 | 10 | 11 | ← | 10 | 1 | 9 | 10 | 21715.0870 | -0.0226 |
| 12 | 1 | 12 | 11 | ← | 11 | 1 | 11 | 10 | 21795.8075 | 0.0030 |
| 12 | 1 | 12 | 12 | ← | 11 | 1 | 11 | 11 | 21795.8075 | -0.0018 |
| 12 | 1 | 12 | 13 | ← | 11 | 1 | 11 | 12 | 21795.8075 | -0.0069 |
| 12 | 0 | 12 | 11 | ← | 11 | 0 | 11 | 10 | 21886.4033 | 0.0280 |
| 12 | 0 | 12 | 13 | ← | 11 | 0 | 11 | 12 | 21886.4033 | 0.0173 |
| 12 | 0 | 12 | 12 | ← | 11 | 0 | 11 | 11 | 21886.4033 | 0.0152 |
| 11 | 2 | 9 | 11 | ← | 10 | 2 | 8 | 10 | 22240.7705 | 0.0095 |

| J' | $K_{a'}$ | $K_{c'}$ | F' | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | 2 | 9 | 10 | ← | 10 | 2 | 8 | 9 | 22240.7705 | -0.0128 |
| 11 | 2 | 9 | 12 | ← | 10 | 2 | 8 | 11 | 22240.7705 | -0.0232 |
| 12 | 1 | 11 | 11 | ← | 11 | 1 | 10 | 10 | 23531.8329 | 0.0156 |
| 12 | 1 | 11 | 13 | ← | 11 | 1 | 10 | 12 | 23531.8329 | 0.0035 |
| 12 | 1 | 11 | 12 | ← | 11 | 1 | 10 | 11 | 23531.8329 | -0.0056 |
| | | | | | | | | | RMS | 11.0 kHz |

Table S18 Linelist for $^{13}$C3 isotopologue of Conformer I of isoleucinol. OMC is the difference between the observed and calculated transition.

| J' | $K_{a'}$ | $K_{c'}$ | F' | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 0 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 3872.2532 | 0.0013 |
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 5543.5047 | 0.0017 |
| 3 | 1 | 3 | 2 | ← | 2 | 1 | 2 | 1 | 5543.5047 | -0.0049 |
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 1 | 5785.9225 | -0.0084 |
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 5786.1850 | -0.0095 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 7381.3272 | 0.0025 |
| 4 | 1 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 7381.4826 | -0.0044 |
| 4 | 0 | 4 | 3 | ← | 3 | 0 | 3 | 2 | 7674.3224 | -0.0003 |
| 4 | 0 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 7674.4416 | -0.0056 |
| 4 | 0 | 4 | 3 | ← | 3 | 0 | 3 | 3 | 7676.1974 | 0.0031 |
| 4 | 2 | 3 | 4 | ← | 3 | 2 | 2 | 4 | 7754.7618 | 0.0044 |
| 4 | 2 | 3 | 5 | ← | 3 | 2 | 2 | 4 | 7755.3424 | 0.0122 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 2 | 7755.4863 | 0.0088 |
| 4 | 2 | 2 | 4 | ← | 3 | 2 | 1 | 3 | 7842.4360 | 0.0060 |
| 4 | 2 | 2 | 5 | ← | 3 | 2 | 1 | 4 | 7843.0249 | 0.0067 |
| 4 | 2 | 2 | 3 | ← | 3 | 2 | 1 | 2 | 7843.1672 | -0.0003 |
| 4 | 1 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 8107.2161 | -0.0030 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 9530.8289 | -0.0208 |
| 5 | 0 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 9530.8289 | -0.0247 |
| 5 | 1 | 4 | 6 | ← | 4 | 1 | 3 | 5 | 10115.4193 | 0.0000 |
| 6 | 0 | 6 | 7 | ← | 5 | 0 | 5 | 6 | 11352.8810 | -0.0173 |
| 6 | 0 | 6 | 6 | ← | 5 | 0 | 5 | 5 | 11352.8810 | -0.0203 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 18233.2954 | 0.0013 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 18233.2954 | -0.0029 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 18233.2954 | -0.0128 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 18398.4481 | 0.0001 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 18398.4481 | -0.0160 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 18398.4481 | -0.0212 |
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 8 | 19184.9704 | 0.0069 |
| 10 | 2 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 19184.9704 | -0.0039 |
| 10 | 1 | 9 | 9 | ← | 9 | 1 | 8 | 8 | 19855.0266 | 0.0027 |
| 10 | 1 | 9 | 11 | ← | 9 | 1 | 8 | 10 | 19855.0266 | -0.0140 |
| 10 | 1 | 9 | 10 | ← | 9 | 1 | 8 | 9 | 19855.0266 | -0.0143 |
| 11 | 1 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 20014.1851 | -0.0279 |
| 11 | 0 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 20138.4529 | 0.0316 |
| 11 | 0 | 11 | 11 | ← | 10 | 0 | 10 | 10 | 20138.4529 | 0.0281 |
| 11 | 1 | 10 | 10 | ← | 10 | 1 | 9 | 9 | 21709.3005 | -0.0087 |
| 11 | 1 | 10 | 12 | ← | 10 | 1 | 9 | 11 | 21709.3005 | -0.0230 |
| 11 | 1 | 10 | 11 | ← | 10 | 1 | 9 | 10 | 21709.3005 | -0.0285 |
| 12 | 1 | 12 | 12 | ← | 11 | 1 | 11 | 11 | 21789.5636 | -0.0009 |
| 12 | 1 | 12 | 13 | ← | 11 | 1 | 11 | 12 | 21789.5636 | -0.0059 |
| 12 | 0 | 12 | 11 | ← | 11 | 0 | 11 | 10 | 21880.1477 | 0.0071 |
| 12 | 0 | 12 | 13 | ← | 11 | 0 | 11 | 12 | 21880.1477 | -0.0035 |
| 12 | 0 | 12 | 12 | ← | 11 | 0 | 11 | 11 | 21880.1477 | -0.0056 |
| 11 | 2 | 9 | 11 | ← | 10 | 2 | 8 | 10 | 22234.9031 | 0.0079 |
| 11 | 2 | 9 | 10 | ← | 10 | 2 | 8 | 9 | 22234.9031 | -0.0145 |
| 11 | 2 | 9 | 12 | ← | 10 | 2 | 8 | 11 | 22234.9031 | -0.0248 |
| 12 | 2 | 11 | 11 | ← | 11 | 2 | 10 | 10 | 22902.9257 | 0.0186 |
| 12 | 2 | 11 | 13 | ← | 11 | 2 | 10 | 12 | 22902.9257 | 0.0098 |
| 13 | 0 | 13 | 12 | ← | 12 | 0 | 12 | 11 | 23624.9504 | 0.0213 |
| 13 | 0 | 13 | 14 | ← | 12 | 0 | 12 | 13 | 23624.9504 | 0.0124 |
| 13 | 0 | 13 | 13 | ← | 12 | 0 | 12 | 12 | 23624.9504 | 0.0114 |
| 13 | 1 | 12 | 14 | ← | 12 | 1 | 11 | 13 | 25306.5783 | 0.0269 |
| 13 | 1 | 12 | 13 | ← | 12 | 1 | 11 | 12 | 25306.5783 | 0.0156 |
| | | | | | | | | | RMS | 12.2 kHz |

Table S19 Linelist for $^{13}$C4 isotopologue of Conformer I of isoleucinol. OMC is the difference between the observed and calculated transition.

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 0 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 3849.3556 | 0.0042 |
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 5511.8251 | 0.0050 |
| 3 | 2 | 2 | 3 | ← | 2 | 2 | 1 | 2 | 5785.9221 | 0.0022 |
| 3 | 2 | 2 | 2 | ← | 2 | 2 | 1 | 2 | 5785.9221 | 0.0018 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 6051.0670 | 0.0002 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6051.4451 | 0.0014 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 7339.2545 | -0.0059 |
| 4 | 1 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 7339.4093 | -0.0135 |
| 4 | 0 | 4 | 3 | ← | 3 | 0 | 3 | 2 | 7629.8257 | 0.0000 |
| 4 | 0 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 7629.9404 | -0.0098 |
| 4 | 2 | 2 | 4 | ← | 3 | 2 | 1 | 3 | 7794.7898 | 0.0073 |
| 4 | 2 | 2 | 5 | ← | 3 | 2 | 1 | 4 | 7795.3785 | 0.0078 |
| 4 | 1 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 8057.6697 | -0.0136 |
| 5 | 0 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 9476.3330 | -0.0057 |
| 5 | 1 | 4 | 6 | ← | 4 | 1 | 3 | 5 | 10053.8704 | 0.0027 |
| 6 | 0 | 6 | 7 | ← | 5 | 0 | 5 | 6 | 11288.8709 | -0.0004 |
| 6 | 0 | 6 | 6 | ← | 5 | 0 | 5 | 5 | 11288.8709 | -0.0034 |
| 6 | 2 | 5 | 5 | ← | 5 | 2 | 4 | 4 | 11534.7787 | -0.0041 |
| 6 | 2 | 5 | 7 | ← | 5 | 2 | 4 | 6 | 11534.7787 | -0.0048 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 18131.6700 | 0.0024 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 18131.6700 | -0.0017 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 18131.6700 | -0.0116 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 18297.7644 | 0.0175 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 18297.7644 | 0.0014 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 18297.7644 | -0.0038 |
| 10 | 2 | 9 | 10 | ← | 9 | 2 | 8 | 9 | 19073.7224 | 0.0323 |
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 8 | 19073.7224 | 0.0072 |
| 10 | 2 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 19073.7224 | -0.0035 |
| 10 | 1 | 9 | 11 | ← | 9 | 1 | 8 | 10 | 19739.7305 | 0.0206 |
| 10 | 1 | 9 | 10 | ← | 9 | 1 | 8 | 9 | 19739.7305 | 0.0205 |
| 11 | 1 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 19902.9906 | 0.0186 |
| 11 | 1 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 19902.9906 | 0.0138 |
| 11 | 1 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 19902.9906 | 0.0068 |
| 11 | 0 | 11 | 10 | ← | 10 | 0 | 10 | 9 | 20028.2319 | 0.0100 |
| 11 | 0 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 20028.2319 | -0.0030 |
| 11 | 0 | 11 | 11 | ← | 10 | 0 | 10 | 10 | 20028.2319 | -0.0066 |
| 11 | 1 | 10 | 10 | ← | 10 | 1 | 9 | 9 | 21585.0455 | 0.0057 |
| 11 | 1 | 10 | 12 | ← | 10 | 1 | 9 | 11 | 21585.0455 | -0.0085 |
| 11 | 1 | 10 | 11 | ← | 10 | 1 | 9 | 10 | 21585.0455 | -0.0137 |
| 12 | 0 | 12 | 11 | ← | 11 | 0 | 11 | 10 | 21760.3679 | 0.0269 |
| 12 | 0 | 12 | 13 | ← | 11 | 0 | 11 | 12 | 21760.3679 | 0.0162 |
| 12 | 0 | 12 | 12 | ← | 11 | 0 | 11 | 11 | 21760.3679 | 0.0140 |
| 11 | 2 | 9 | 11 | ← | 10 | 2 | 8 | 10 | 22097.5737 | 0.0004 |
| 11 | 2 | 9 | 10 | ← | 10 | 2 | 8 | 9 | 22097.5737 | -0.0221 |
| 12 | 1 | 11 | 11 | ← | 11 | 1 | 10 | 10 | 23392.8427 | 0.0006 |
| 12 | 1 | 11 | 13 | ← | 11 | 1 | 10 | 12 | 23392.8427 | -0.0115 |
| 12 | 1 | 11 | 12 | ← | 11 | 1 | 10 | 11 | 23392.8427 | -0.0205 |
| 13 | 1 | 13 | 12 | ← | 12 | 1 | 12 | 11 | 23430.0469 | -0.0083 |
| 13 | 1 | 13 | 13 | ← | 12 | 1 | 12 | 12 | 23430.0469 | -0.0132 |
| 13 | 1 | 13 | 14 | ← | 12 | 1 | 12 | 13 | 23430.0469 | -0.0169 |
| | | | | | | | | | RMS | 9.2 |

Table S20 Linelist for $^{13}$C5 isotopologue of Conformer I of isoleucinol. OMC is the difference between the observed and calculated transition.

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 5443.4102 | -0.0050 |
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 5443.7868 | 0.0002 |
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 1 | 5678.5030 | -0.0060 |
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 5678.7605 | -0.0121 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 5968.6261 | 0.0067 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 7249.1072 | 0.0010 |
| 4 | 1 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 7249.2672 | -0.0015 |
| 4 | 0 | 4 | 3 | ← | 3 | 0 | 3 | 2 | 7534.1595 | -0.0047 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 7534.2851 | 0.0137 |
| 4 | 2 | 3 | 4 | ← | 3 | 2 | 2 | 3 | 7608.4005 | 0.0002 |
| 4 | 2 | 3 | 4 | ← | 3 | 2 | 2 | 4 | 7608.4005 | 0.0001 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 2 | 7609.1248 | 0.0043 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 3 | 7609.1248 | 0.0038 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 4 | 7609.1248 | 0.0037 |
| 4 | 3 | 2 | 4 | ← | 3 | 3 | 1 | 3 | 7629.9405 | -0.0039 |
| 5 | 1 | 5 | 5 | ← | 4 | 1 | 4 | 4 | 9047.6211 | -0.0226 |
| 5 | 1 | 5 | 6 | ← | 4 | 1 | 4 | 5 | 9047.7509 | 0.0207 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 9360.1614 | -0.0069 |
| 5 | 0 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 9360.1614 | -0.0116 |
| 5 | 2 | 3 | 6 | ← | 4 | 2 | 2 | 5 | 9659.6639 | -0.0164 |
| 5 | 1 | 4 | 5 | ← | 4 | 1 | 3 | 4 | 9918.3475 | -0.0125 |
| 5 | 1 | 4 | 6 | ← | 4 | 1 | 3 | 5 | 9918.4680 | 0.0202 |
| 6 | 1 | 6 | 6 | ← | 5 | 1 | 5 | 5 | 10838.1407 | -0.0147 |
| 6 | 0 | 6 | 7 | ← | 5 | 0 | 5 | 6 | 11153.7160 | 0.0085 |
| 6 | 0 | 6 | 6 | ← | 5 | 0 | 5 | 5 | 11153.7160 | 0.0058 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 18089.0359 | 0.0230 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 18089.0359 | 0.0175 |
| 10 | 1 | 9 | 9 | ← | 9 | 1 | 8 | 8 | 19493.4075 | -0.0057 |
| 10 | 1 | 9 | 10 | ← | 9 | 1 | 8 | 9 | 19493.4075 | -0.0221 |
| 10 | 1 | 9 | 11 | ← | 9 | 1 | 8 | 10 | 19493.4075 | -0.0236 |
| 11 | 1 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 19668.3568 | 0.0065 |
| 11 | 1 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 19668.3568 | 0.0018 |
| 11 | 1 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 19668.3568 | -0.0052 |
| 11 | 0 | 11 | 10 | ← | 10 | 0 | 10 | 9 | 19799.5761 | 0.0073 |
| 11 | 0 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 19799.5761 | -0.0057 |
| 11 | 0 | 11 | 11 | ← | 10 | 0 | 10 | 10 | 19799.5761 | -0.0096 |
| 11 | 2 | 10 | 12 | ← | 10 | 2 | 9 | 11 | 20668.8780 | 0.0310 |
| 11 | 1 | 10 | 10 | ← | 10 | 1 | 9 | 9 | 21322.3027 | -0.0261 |
| 12 | 1 | 12 | 11 | ← | 11 | 1 | 11 | 10 | 21414.2757 | 0.0041 |
| 12 | 1 | 12 | 12 | ← | 11 | 1 | 11 | 11 | 21414.2757 | -0.0007 |
| 12 | 1 | 12 | 13 | ← | 11 | 1 | 11 | 12 | 21414.2757 | -0.0058 |
| 12 | 0 | 12 | 13 | ← | 11 | 0 | 11 | 12 | 21511.3207 | 0.0252 |
| 12 | 0 | 12 | 12 | ← | 11 | 0 | 11 | 11 | 21511.3207 | 0.0227 |
| 11 | 2 | 9 | 11 | ← | 10 | 2 | 8 | 10 | 21791.6245 | 0.0239 |
| 11 | 2 | 9 | 10 | ← | 10 | 2 | 8 | 9 | 21791.6245 | 0.0004 |
| 11 | 2 | 9 | 12 | ← | 10 | 2 | 8 | 11 | 21791.6245 | -0.0098 |
| 12 | 2 | 11 | 11 | ← | 11 | 2 | 10 | 10 | 22490.8822 | 0.0307 |
| 12 | 2 | 11 | 13 | ← | 11 | 2 | 10 | 12 | 22490.8822 | 0.0220 |
| 13 | 1 | 13 | 12 | ← | 12 | 1 | 12 | 11 | 23155.7128 | -0.0098 |
| 13 | 1 | 13 | 13 | ← | 12 | 1 | 12 | 12 | 23155.7128 | -0.0146 |
| 13 | 1 | 13 | 14 | ← | 12 | 1 | 12 | 13 | 23155.7128 | -0.0183 |
| 13 | 0 | 13 | 13 | ← | 12 | 0 | 12 | 12 | 23225.6945 | -0.0242 |
| 13 | 0 | 13 | 12 | ← | 12 | 0 | 12 | 11 | 23225.6945 | -0.0139 |
| 13 | 0 | 13 | 14 | ← | 12 | 0 | 12 | 13 | 23225.6945 | -0.0229 |
| | | | | | | | | | RMS | 14.7 kHz |

Table S21 Linelist for $^{13}$C6 isotopologue of Conformer I of isoleucinol. OMC is the difference between the observed and calculated transition.

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 0 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 3859.6615 | 0.0096 |
| 2 | 0 | 2 | 1 | ← | 1 | 0 | 1 | 1 | 3861.6593 | -0.0057 |
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 5518.6191 | 0.0004 |
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 5765.5427 | -0.0124 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 6076.7109 | 0.0118 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6077.0916 | 0.0159 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 7347.4059 | 0.0011 |
| 4 | 1 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 7347.5545 | -0.0123 |
| 4 | 0 | 4 | 3 | ← | 3 | 0 | 3 | 2 | 7643.7183 | 0.0053 |
| 4 | 0 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 7643.8389 | 0.0012 |
| 4 | 1 | 3 | 4 | ← | 3 | 1 | 2 | 3 | 8090.5658 | 0.0018 |
| 4 | 1 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 8090.7201 | -0.0089 |
| 5 | 1 | 5 | 6 | ← | 4 | 1 | 4 | 5 | 9168.4363 | 0.0144 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 9488.1386 | -0.0096 |

| J' | $K_{a'}$ | $K_{c'}$ | F' | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | 0 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 9488.1386 | -0.0124 |
| 5 | 1 | 4 | 5 | ← | 4 | 1 | 3 | 5 | 10091.8238 | -0.0103 |
| 5 | 1 | 4 | 6 | ← | 4 | 1 | 3 | 5 | 10093.2193 | -0.0007 |
| 6 | 1 | 6 | 6 | ← | 5 | 1 | 5 | 5 | 10980.0992 | -0.0227 |
| 6 | 0 | 6 | 7 | ← | 5 | 0 | 5 | 6 | 11296.3627 | -0.0096 |
| 6 | 0 | 6 | 6 | ← | 5 | 0 | 5 | 5 | 11296.3627 | -0.0142 |
| 6 | 2 | 5 | 5 | ← | 5 | 2 | 4 | 4 | 11564.3751 | -0.0119 |
| 9 | 2 | 7 | 8 | ← | 8 | 2 | 6 | 7 | 18086.8738 | -0.0018 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 18135.2995 | 0.0147 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 18135.2995 | 0.0103 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 18135.2995 | 0.0006 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 18288.5914 | 0.0210 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 18288.5914 | 0.0049 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 18288.5914 | 0.0001 |
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 8 | 19108.5469 | 0.0168 |
| 10 | 2 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 19108.5469 | 0.0060 |
| 10 | 1 | 9 | 9 | ← | 9 | 1 | 8 | 8 | 19776.4706 | 0.0063 |
| 10 | 1 | 9 | 11 | ← | 9 | 1 | 8 | 10 | 19776.4706 | -0.0105 |
| 10 | 1 | 9 | 10 | ← | 9 | 1 | 8 | 9 | 19776.4706 | -0.0121 |
| 11 | 1 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 19904.7070 | 0.0170 |
| 11 | 1 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 19904.7070 | 0.0121 |
| 11 | 1 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 19904.7070 | 0.0052 |
| 11 | 0 | 11 | 10 | ← | 10 | 0 | 10 | 9 | 20018.0172 | 0.0163 |
| 11 | 0 | 11 | 12 | ← | 10 | 0 | 10 | 11 | 20018.0172 | 0.0034 |
| 11 | 0 | 11 | 11 | ← | 10 | 0 | 10 | 10 | 20018.0172 | 0.0003 |
| 10 | 2 | 8 | 10 | ← | 9 | 2 | 7 | 9 | 20151.8053 | -0.0081 |
| 11 | 2 | 10 | 10 | ← | 10 | 2 | 9 | 9 | 20962.6703 | 0.0201 |
| 11 | 2 | 10 | 12 | ← | 10 | 2 | 9 | 11 | 20962.6703 | 0.0103 |
| 11 | 1 | 10 | 10 | ← | 10 | 1 | 9 | 9 | 21611.9153 | -0.0056 |
| 11 | 1 | 10 | 12 | ← | 10 | 1 | 9 | 11 | 21611.9153 | -0.0199 |
| 11 | 1 | 10 | 11 | ← | 10 | 1 | 9 | 10 | 21611.9153 | -0.0266 |
| 12 | 0 | 12 | 13 | ← | 11 | 0 | 11 | 12 | 21749.8651 | -0.0032 |
| 12 | 0 | 12 | 12 | ← | 11 | 0 | 11 | 11 | 21749.8651 | -0.0048 |
| 12 | 1 | 11 | 11 | ← | 11 | 1 | 10 | 10 | 23407.8142 | 0.0219 |
| 12 | 1 | 11 | 13 | ← | 11 | 1 | 10 | 12 | 23407.8142 | 0.0097 |
| 12 | 1 | 11 | 12 | ← | 11 | 1 | 10 | 11 | 23407.8142 | -0.0004 |
| 13 | 1 | 13 | 12 | ← | 12 | 1 | 12 | 11 | 23428.1388 | 0.0160 |
| 13 | 1 | 13 | 13 | ← | 12 | 1 | 12 | 12 | 23428.1388 | 0.0112 |
| 13 | 1 | 13 | 14 | ← | 12 | 1 | 12 | 13 | 23428.1388 | 0.0075 |
| 13 | 0 | 13 | 12 | ← | 12 | 0 | 12 | 11 | 23485.0498 | -0.0082 |
| 13 | 0 | 13 | 14 | ← | 12 | 0 | 12 | 13 | 23485.0498 | -0.0171 |
| 13 | 0 | 13 | 13 | ← | 12 | 0 | 12 | 12 | 23485.0498 | -0.0177 |
| | | | | | | | | | RMS | 10.7 kHz |

Table S22 Linelist for $^{18}O$ isotopologue of Conformer I of isoleucinol. OMC is the difference between the observed and calculated transition.

| J' | $K_{a'}$ | $K_{c'}$ | F' | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | 1 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 7149.6592 | -0.0011 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 7428.5044 | 0.0051 |
| 4 | 1 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 7828.5039 | -0.0010 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 9231.3459 | -0.0039 |
| 5 | 0 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 9231.3459 | -0.0093 |
| | | | | | | | | | RMS | 4.3 kHz |

Table S23 Linelist for $^{15}N$ isotopologue of Conformer I of isoleucinol. OMC is the difference between the observed and calculated transition.

| J' | $K_{a'}$ | $K_{c'}$ | | J | $K_a$ | $K_c$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|
| 3 | 0 | 3 | ← | 2 | 0 | 2 | 5768.4432 | -0.0006 |
| 3 | 1 | 2 | ← | 2 | 1 | 1 | 6078.0275 | 0.0047 |
| 4 | 1 | 4 | ← | 3 | 1 | 3 | 7352.7788 | 0.0136 |
| 4 | 0 | 4 | ← | 3 | 0 | 3 | 7648.3660 | -0.0007 |
| 4 | 2 | 2 | ← | 3 | 2 | 1 | 7827.1782 | -0.0010 |
| 5 | 1 | 5 | ← | 4 | 1 | 4 | 9175.1813 | -0.0018 |
| 5 | 0 | 5 | ← | 4 | 0 | 4 | 9494.7657 | 0.0163 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | | $J$ | $K_a$ | $K_c$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|
| 5 | 1 | 4 | ← | 4 | 1 | 3 | 10095.5170 | -0.0050 |
| 6 | 1 | 6 | ← | 5 | 1 | 5 | 10988.5807 | -0.0179 |
| 6 | 0 | 6 | ← | 5 | 0 | 5 | 11305.3949 | 0.0082 |
| 10 | 0 | 10 | ← | 9 | 0 | 9 | 18306.7969 | 0.0176 |
| 10 | 1 | 9 | ← | 9 | 1 | 8 | 19788.2809 | -0.0031 |
| 11 | 1 | 11 | ← | 10 | 1 | 10 | 19922.4782 | -0.0239 |
| 11 | 1 | 10 | ← | 10 | 1 | 9 | 21627.1744 | -0.0097 |
| | | | | | | | RMS | 11.6 kHz |

## S7.2 Isotopologues of Conformers II

Table S24 Linelist for $^{13}$C1 isotopologue of Conformer II of isoleucinol. OMC is the difference between the observed and calculated transition.

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6383.8884 | -0.0009 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 6383.5113 | -0.0036 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 7978.1045 | 0.0029 |
| 4 | 1 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 7978.2787 | 0.0059 |
| 5 | 0 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 10198.0351 | 0.0142 |
| 9 | 0 | 9 | 10 | ← | 8 | 0 | 8 | 9 | 18001.9730 | -0.0127 |
| 9 | 0 | 9 | 9 | ← | 8 | 0 | 8 | 8 | 18001.9730 | 0.0049 |
| 9 | 0 | 9 | 8 | ← | 8 | 0 | 8 | 7 | 18001.9730 | 0.0072 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 19790.9912 | -0.0185 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 19921.8802 | 0.0075 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 19921.8802 | -0.0081 |
| | | | | | | | | | RMS | 8.7 kHz |

Table S25 Linelist for $^{13}$C2 isotopologue of Conformer II of isoleucinol. OMC is the difference between the observed and calculated transition.

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 6016.3231 | 0.0010 |
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 6193.5389 | -0.0061 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6412.0952 | -0.0017 |
| 3 | 1 | 2 | 2 | ← | 2 | 1 | 1 | 1 | 6412.0952 | -0.0101 |
| 4 | 1 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 8014.9224 | 0.0068 |
| 4 | 0 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 8230.0529 | -0.0174 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 8230.0529 | 0.0212 |
| 4 | 1 | 3 | 4 | ← | 3 | 1 | 2 | 3 | 8541.6122 | -0.0069 |
| 5 | 0 | 5 | 4 | ← | 4 | 0 | 4 | 3 | 10244.3538 | 0.0186 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 10244.3538 | -0.0224 |
| 9 | 0 | 9 | 9 | ← | 8 | 0 | 8 | 8 | 18085.0624 | 0.0002 |
| 9 | 0 | 9 | 10 | ← | 8 | 0 | 8 | 9 | 18085.0624 | -0.0174 |
| 9 | 1 | 8 | 8 | ← | 8 | 1 | 7 | 7 | 19029.3944 | 0.0127 |
| 9 | 1 | 8 | 10 | ← | 8 | 1 | 7 | 9 | 19029.3944 | -0.0037 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 19882.5115 | -0.0043 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 19882.5115 | -0.0013 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 19882.5115 | -0.0200 |
| 10 | 2 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 20574.1264 | 0.0207 |
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 8 | 20574.1264 | 0.0310 |
| | | | | | | | | | RMS | 9.6 kHz |

Table S26 Linelist for $^{13}$C3 isotopologue of Conformer II of isoleucinol. OMC is the difference between the observed and calculated transition.

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 6015.9087 | 0.0090 |
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 6192.1825 | -0.0046 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 6408.9672 | 0.0013 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6409.3448 | 0.0045 |
| 3 | 1 | 2 | 2 | ← | 2 | 1 | 1 | 1 | 6409.3448 | -0.0038 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | 1 | 4 | 3 | ← | 3 | 1 | 3 | 2 | 8014.3660 | 0.0017 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 10242.9553 | -0.0024 |
| 5 | 1 | 4 | 6 | ← | 4 | 1 | 3 | 5 | 10660.1398 | 0.0221 |
| 9 | 1 | 8 | 9 | ← | 8 | 1 | 7 | 8 | 19023.6529 | 0.0202 |
| 9 | 1 | 8 | 8 | ← | 8 | 1 | 7 | 7 | 19023.6529 | 0.0116 |
| 9 | 1 | 8 | 10 | ← | 8 | 1 | 7 | 9 | 19023.6529 | -0.0048 |
| 9 | 2 | 7 | 8 | ← | 8 | 2 | 6 | 7 | 19100.8876 | -0.0150 |
| 9 | 2 | 7 | 10 | ← | 8 | 2 | 6 | 9 | 19100.8876 | -0.0265 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 19882.7715 | 0.0062 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 19882.7715 | 0.0032 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 19882.7715 | -0.0125 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 20014.7343 | -0.0062 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 20014.7343 | -0.0066 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 20014.7343 | -0.0223 |
| 10 | 2 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 20570.3594 | 0.0094 |
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 8 | 20570.3594 | 0.0197 |
| 10 | 1 | 9 | 10 | ← | 9 | 1 | 8 | 9 | 21066.8491 | -0.0098 |
| 10 | 1 | 9 | 9 | ← | 9 | 1 | 8 | 8 | 21066.8491 | -0.0177 |
| | | | | | | | | | RMS | 11.3 kHz |

Table S27 Linelist for $^{13}$C4 isotopologue of Conformer II of isoleucinol. OMC is the difference between the observed and calculated transition.

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 5993.4474 | -0.0074 |
| 3 | 1 | 3 | 2 | ← | 2 | 1 | 2 | 1 | 5993.4474 | 0.0159 |
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 6169.5284 | -0.0005 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 6386.1181 | 0.0005 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6386.4908 | -0.0012 |
| 3 | 1 | 2 | 2 | ← | 2 | 1 | 1 | 1 | 6386.4908 | -0.0096 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 7984.3230 | -0.0025 |
| 4 | 1 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 7984.4970 | 0.0002 |
| 4 | 0 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 8198.3556 | 0.0122 |
| 4 | 1 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 8507.7251 | -0.0043 |
| 5 | 0 | 5 | 4 | ← | 4 | 0 | 4 | 3 | 10205.1255 | 0.0069 |
| 9 | 0 | 9 | 9 | ← | 8 | 0 | 8 | 8 | 18017.4819 | 0.0082 |
| 9 | 0 | 9 | 10 | ← | 8 | 0 | 8 | 9 | 18017.4819 | -0.0094 |
| 9 | 2 | 8 | 9 | ← | 8 | 2 | 7 | 8 | 18472.8894 | 0.0283 |
| 9 | 2 | 8 | 8 | ← | 8 | 2 | 7 | 7 | 18472.8894 | -0.0198 |
| 9 | 2 | 8 | 10 | ← | 8 | 2 | 7 | 9 | 18472.8894 | -0.0310 |
| 9 | 1 | 8 | 8 | ← | 8 | 1 | 7 | 7 | 18954.9356 | 0.0181 |
| 9 | 1 | 8 | 10 | ← | 8 | 1 | 7 | 9 | 18954.9356 | 0.0016 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 19807.9434 | 0.0125 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 19807.9434 | 0.0095 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 19807.9434 | -0.0062 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 19939.3949 | -0.0057 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 19939.3949 | -0.0062 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 19939.3949 | -0.0219 |
| | | | | | | | | | RMS | 6.4 kHz |

Table S28 Linelist for $^{13}$C5 isotopologue of Conformer II of isoleucinol. OMC is the difference between the observed and calculated transition.

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 6090.6389 | -0.0063 |
| 4 | 1 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 7881.4660 | -0.0033 |
| 5 | 1 | 5 | 6 | ← | 4 | 1 | 4 | 5 | 9841.7804 | 0.0133 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 10075.3016 | 0.0019 |
| 9 | 2 | 8 | 8 | ← | 8 | 2 | 7 | 7 | 18237.0163 | 0.0076 |
| 9 | 2 | 8 | 10 | ← | 8 | 2 | 7 | 9 | 18237.0163 | -0.0035 |
| 9 | 1 | 8 | 10 | ← | 8 | 1 | 7 | 9 | 18716.0027 | 0.0031 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 19686.0698 | 0.0028 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 19686.0698 | -0.0133 |

| J’ | $K_{a'}$ | $K_{c'}$ | F’ | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 19686.0698 | 0.0024 |
| | | | | | | | | | RMS | 6.0 kHz |

Table S29 Linelist for $^{13}$C6 isotopologue of Conformer II of isoleucinol. OMC is the difference between the observed and calculated transition.

| J’ | $K_{a'}$ | $K_{c'}$ | F’ | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 5975.1821 | -0.0143 |
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 5975.5905 | 0.0136 |
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 6155.3634 | 0.0023 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6378.9598 | 0.0020 |
| 3 | 1 | 2 | 2 | ← | 2 | 1 | 1 | 1 | 6378.9598 | -0.0063 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 7960.0221 | -0.0027 |
| 4 | 1 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 7960.1930 | -0.0030 |
| 4 | 1 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 8497.1216 | -0.0007 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 10176.3085 | 0.0052 |
| 9 | 2 | 8 | 10 | ← | 8 | 2 | 7 | 9 | 18427.9760 | 0.0104 |
| 9 | 2 | 8 | 8 | ← | 8 | 2 | 7 | 7 | 18427.9760 | 0.0216 |
| 9 | 1 | 8 | 8 | ← | 8 | 1 | 7 | 7 | 18915.8618 | 0.0020 |
| 9 | 1 | 8 | 10 | ← | 8 | 1 | 7 | 9 | 18915.8618 | -0.0144 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 19863.3429 | 0.0069 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 19863.3429 | -0.0087 |
| 10 | 1 | 9 | 10 | ← | 9 | 1 | 8 | 9 | 20941.2775 | -0.0014 |
| | | | | | | | | | RMS | 7.9 kHz |

### S7.3 Isotopologues of Conformers III

Table S30 Linelist for $^{13}$C1 isotopologue of Conformer III of isoleucinol. OMC is the difference between the observed and calculated transition.

| J’ | $K_{a'}$ | $K_{c'}$ | F’ | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 6313.6046 | -0.0141 |
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 6563.4096 | 0.0112 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 6915.7704 | 0.0026 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6916.0862 | 0.0083 |
| 4 | 0 | 4 | 3 | ← | 3 | 0 | 3 | 2 | 8683.3358 | 0.0042 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 8683.4512 | 0.0176 |
| 4 | 2 | 3 | 5 | ← | 3 | 2 | 2 | 4 | 8820.8802 | 0.0062 |
| 4 | 1 | 3 | 3 | ← | 3 | 1 | 2 | 2 | 9201.4244 | -0.0253 |
| 5 | 1 | 5 | 5 | ← | 4 | 1 | 4 | 4 | 10478.2418 | -0.0078 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 10756.0515 | -0.0164 |
| 6 | 0 | 6 | 7 | ← | 5 | 0 | 5 | 6 | 12786.5629 | 0.0200 |
| 6 | 0 | 6 | 6 | ← | 5 | 0 | 5 | 5 | 12786.5629 | 0.0092 |
| 8 | 1 | 7 | 7 | ← | 7 | 1 | 6 | 6 | 18069.6667 | 0.0150 |
| 8 | 1 | 7 | 8 | ← | 7 | 1 | 6 | 7 | 18069.6667 | -0.0049 |
| 8 | 1 | 7 | 9 | ← | 7 | 1 | 6 | 8 | 18069.6667 | -0.0066 |
| 8 | 2 | 6 | 8 | ← | 7 | 2 | 5 | 7 | 18358.2621 | 0.0074 |
| 9 | 1 | 9 | 9 | ← | 8 | 1 | 8 | 8 | 18664.1509 | 0.0061 |
| 9 | 1 | 9 | 10 | ← | 8 | 1 | 8 | 9 | 18664.1509 | -0.0037 |
| 9 | 0 | 9 | 9 | ← | 8 | 0 | 8 | 8 | 18764.3736 | 0.0026 |
| 9 | 0 | 9 | 10 | ← | 8 | 0 | 8 | 9 | 18764.3736 | 0.0063 |
| 9 | 0 | 9 | 8 | ← | 8 | 0 | 8 | 7 | 18764.3736 | 0.0224 |
| 9 | 1 | 8 | 8 | ← | 8 | 1 | 7 | 7 | 20177.4013 | 0.0007 |
| 9 | 1 | 8 | 10 | ← | 8 | 1 | 7 | 9 | 20177.4013 | -0.0170 |
| 9 | 1 | 8 | 9 | ← | 8 | 1 | 7 | 8 | 20177.4013 | -0.0244 |
| 9 | 2 | 7 | 8 | ← | 8 | 2 | 6 | 7 | 20690.6056 | -0.0026 |
| 9 | 2 | 7 | 10 | ← | 8 | 2 | 6 | 9 | 20690.6056 | -0.0137 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 20754.1885 | 0.0046 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 20754.1885 | -0.0078 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 20754.1885 | -0.0094 |
| | | | | | | | | | RMS | 11.5 kHz |

Table S31 Linelist for $^{13}$C2 isotopologue of Conformer III of isoleucinol. OMC is the difference between the observed and calculated transition.

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 6355.2814 | -0.0098 |
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 6606.5254 | 0.0136 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 6962.4366 | -0.0047 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6962.7629 | 0.0114 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 8456.8611 | 0.0098 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 8739.7873 | 0.0003 |
| 4 | 0 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 8739.7873 | -0.0018 |
| 4 | 1 | 3 | 5 | ← | 3 | 1 | 2 | 4 | 9263.3396 | -0.0247 |
| 5 | 1 | 5 | 4 | ← | 4 | 1 | 4 | 3 | 10546.5094 | 0.0206 |
| 5 | 1 | 5 | 6 | ← | 4 | 1 | 4 | 5 | 10546.5094 | -0.0146 |
| 5 | 0 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 10825.0078 | -0.0185 |
| 8 | 3 | 5 | 7 | ← | 7 | 3 | 4 | 6 | 18064.2042 | -0.0067 |
| 8 | 3 | 5 | 9 | ← | 7 | 3 | 4 | 8 | 18064.2042 | 0.0000 |
| 8 | 1 | 7 | 7 | ← | 7 | 1 | 6 | 6 | 18186.8345 | 0.0024 |
| 8 | 1 | 7 | 8 | ← | 7 | 1 | 6 | 7 | 18186.8345 | -0.0179 |
| 8 | 1 | 7 | 9 | ← | 7 | 1 | 6 | 8 | 18186.8345 | -0.0192 |
| 8 | 2 | 6 | 8 | ← | 7 | 2 | 5 | 7 | 18484.2022 | 0.0059 |
| 9 | 0 | 9 | 10 | ← | 8 | 0 | 8 | 9 | 18883.3851 | 0.0084 |
| 9 | 0 | 9 | 9 | ← | 8 | 0 | 8 | 8 | 18883.3851 | 0.0047 |
| 9 | 1 | 8 | 8 | ← | 8 | 1 | 7 | 7 | 20306.4700 | 0.0238 |
| 9 | 1 | 8 | 10 | ← | 8 | 1 | 7 | 9 | 20306.4700 | 0.0060 |
| 9 | 1 | 8 | 9 | ← | 8 | 1 | 7 | 8 | 20306.4700 | -0.0016 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 20820.6497 | -0.0171 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 20820.6497 | -0.0238 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 20886.1966 | 0.0196 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 20886.1966 | 0.0071 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 20886.1966 | 0.0057 |
| | | | | | | | | | RMS | 12.1 kHz |

Table S32 Linelist for $^{13}$C3 isotopologue of Conformer III of isoleucinol. OMC is the difference between the observed and calculated transition.

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 0 | 2 | 3 | ← | 1 | 0 | 1 | 2 | 4424.3227 | -0.0107 |
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 6347.3374 | -0.0041 |
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 6347.6479 | 0.0013 |
| 3 | 1 | 3 | 2 | ← | 2 | 1 | 2 | 1 | 6347.6479 | -0.0055 |
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 6597.8743 | 0.0138 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6952.6885 | 0.0078 |
| 4 | 1 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 8446.8591 | 0.0035 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 8446.7166 | -0.0074 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 8728.5338 | 0.0101 |
| 4 | 0 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 8728.5338 | 0.0079 |
| 5 | 1 | 5 | 4 | ← | 4 | 1 | 4 | 3 | 10533.9076 | -0.0194 |
| 5 | 1 | 5 | 5 | ← | 4 | 1 | 4 | 4 | 10533.9076 | 0.0133 |
| 8 | 1 | 7 | 7 | ← | 7 | 1 | 6 | 6 | 18161.4792 | 0.0105 |
| 8 | 1 | 7 | 8 | ← | 7 | 1 | 6 | 7 | 18161.4792 | -0.0098 |
| 8 | 1 | 7 | 9 | ← | 7 | 1 | 6 | 8 | 18161.4792 | -0.0112 |
| 9 | 1 | 9 | 10 | ← | 8 | 1 | 8 | 9 | 18762.4607 | -0.0080 |
| 9 | 1 | 9 | 8 | ← | 8 | 1 | 8 | 7 | 18762.4607 | 0.0059 |
| 9 | 1 | 9 | 9 | ← | 8 | 1 | 8 | 8 | 18762.4607 | 0.0017 |
| 9 | 0 | 9 | 10 | ← | 8 | 0 | 8 | 9 | 18861.1551 | 0.0079 |
| 9 | 0 | 9 | 9 | ← | 8 | 0 | 8 | 8 | 18861.1551 | 0.0042 |
| 9 | 1 | 8 | 8 | ← | 8 | 1 | 7 | 7 | 20278.5346 | 0.0177 |
| 9 | 1 | 8 | 10 | ← | 8 | 1 | 7 | 9 | 20278.5346 | -0.0001 |
| 9 | 1 | 8 | 9 | ← | 8 | 1 | 7 | 8 | 20278.5346 | -0.0077 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 20796.6549 | 0.0364 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 20796.6549 | 0.0316 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 20796.6549 | 0.0249 |
| 10 | 2 | 9 | 10 | ← | 9 | 2 | 8 | 9 | 21822.6483 | -0.0190 |
| 10 | 2 | 9 | 9 | ← | 9 | 2 | 8 | 8 | 21822.6483 | -0.0349 |
| 10 | 2 | 9 | 11 | ← | 9 | 2 | 8 | 10 | 21822.6483 | -0.0441 |

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | 1 | 11 | 10 | ← | 10 | 1 | 10 | 11 | 22825.4191 | -0.0132 |
| | | | | | | | | | RMS | 13.2 kHz |

Table S33 Linelist for $^{13}$C4 isotopologue of Conformer III of isoleucinol. OMC is the difference between the observed and calculated transition.

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 1 | 3 | 3 | ← | 2 | 1 | 2 | 2 | 6302.2747 | -0.0108 |
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 6302.5830 | -0.0077 |
| 3 | 1 | 3 | 2 | ← | 2 | 1 | 2 | 1 | 6302.5830 | -0.0147 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 6898.3992 | -0.0003 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6898.7122 | 0.0023 |
| 4 | 0 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 8667.1333 | 0.0120 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 8667.1333 | 0.0147 |
| 4 | 2 | 3 | 3 | ← | 3 | 2 | 2 | 2 | 8801.8410 | -0.0010 |
| 4 | 1 | 3 | 3 | ← | 3 | 1 | 2 | 2 | 9178.7504 | 0.0107 |
| 5 | 1 | 5 | 4 | ← | 4 | 1 | 4 | 3 | 10460.2891 | 0.0058 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 10737.4291 | -0.0141 |
| 5 | 0 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 10737.4291 | -0.0067 |
| 5 | 2 | 4 | 5 | ← | 4 | 2 | 3 | 4 | 10982.9427 | 0.0107 |
| 5 | 2 | 4 | 6 | ← | 4 | 2 | 3 | 5 | 10983.1635 | -0.0126 |
| 8 | 1 | 7 | 7 | ← | 7 | 1 | 6 | 6 | 18032.1576 | 0.0070 |
| 8 | 1 | 7 | 8 | ← | 7 | 1 | 6 | 7 | 18032.1576 | -0.0126 |
| 8 | 1 | 7 | 9 | ← | 7 | 1 | 6 | 8 | 18032.1576 | -0.0146 |
| 9 | 0 | 9 | 8 | ← | 8 | 0 | 8 | 7 | 18736.7130 | 0.0083 |
| 9 | 0 | 9 | 10 | ← | 8 | 0 | 8 | 9 | 18736.7130 | -0.0076 |
| 9 | 0 | 9 | 9 | ← | 8 | 0 | 8 | 8 | 18736.7130 | -0.0115 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 20655.8070 | 0.0180 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 20655.8070 | 0.0247 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 20655.8070 | 0.0295 |
| | | | | | | | | | RMS | 10.7 kHz |

Table S34 Linelist for $^{13}$C5 isotopologue of Conformer III of isoleucinol. OMC is the difference between the observed and calculated transition.

| $J'$ | $K_{a'}$ | $K_{c'}$ | $F'$ | | $J$ | $K_a$ | $K_c$ | $F$ | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 0 | 3 | 2 | ← | 2 | 0 | 2 | 1 | 6512.8046 | 0.0063 |
| 3 | 1 | 2 | 3 | ← | 2 | 1 | 1 | 2 | 6856.0233 | -0.0100 |
| 3 | 1 | 2 | 2 | ← | 2 | 1 | 1 | 1 | 6856.3350 | 0.0140 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6856.3350 | -0.0086 |
| 4 | 1 | 4 | 4 | ← | 3 | 1 | 3 | 3 | 8342.0890 | 0.0098 |
| 4 | 1 | 4 | 5 | ← | 3 | 1 | 3 | 4 | 8342.2127 | 0.0018 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 8619.0346 | 0.0089 |
| 4 | 0 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 8619.0346 | 0.0059 |
| 4 | 2 | 3 | 4 | ← | 3 | 2 | 2 | 3 | 8750.2489 | -0.0059 |
| 4 | 2 | 3 | 4 | ← | 3 | 2 | 2 | 4 | 8750.2489 | -0.0059 |
| 4 | 2 | 3 | 5 | ← | 3 | 2 | 2 | 4 | 8750.7347 | 0.0070 |
| 5 | 0 | 5 | 6 | ← | 4 | 0 | 4 | 5 | 10679.2335 | 0.0157 |
| 5 | 0 | 5 | 5 | ← | 4 | 0 | 4 | 4 | 10679.2335 | 0.0085 |
| 5 | 1 | 4 | 5 | ← | 4 | 1 | 3 | 4 | 11370.7177 | -0.0004 |
| 9 | 1 | 9 | 8 | ← | 8 | 1 | 8 | 7 | 18537.7903 | 0.0207 |
| 9 | 1 | 9 | 9 | ← | 8 | 1 | 8 | 8 | 18537.7903 | 0.0166 |
| 9 | 1 | 9 | 10 | ← | 8 | 1 | 8 | 9 | 18537.7903 | 0.0067 |
| 9 | 2 | 8 | 9 | ← | 8 | 2 | 7 | 8 | 19456.4249 | 0.0257 |
| 9 | 2 | 8 | 8 | ← | 8 | 2 | 7 | 7 | 19456.4249 | -0.0022 |
| 9 | 2 | 8 | 10 | ← | 8 | 2 | 7 | 9 | 19456.4249 | -0.0122 |
| 9 | 1 | 8 | 9 | ← | 8 | 1 | 7 | 8 | 20024.5698 | -0.0142 |
| 9 | 1 | 8 | 8 | ← | 8 | 1 | 7 | 7 | 20024.5698 | 0.0102 |
| 9 | 1 | 8 | 10 | ← | 8 | 1 | 7 | 9 | 20024.5698 | -0.0075 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 20548.6187 | -0.0198 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 20548.6187 | -0.0246 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 20548.6187 | -0.0313 |
| 10 | 0 | 10 | 9 | ← | 9 | 0 | 9 | 8 | 20617.0587 | 0.0022 |

| J' | $K_{a'}$ | $K_{c'}$ | F' | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 20617.0587 | -0.0103 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 20617.0587 | -0.0120 |
| | | | | | | | | | RMS | 9.9 kHz |

Table S35 Linelist for $^{13}$C6 isotopologue of Conformer III of isoleucinol. OMC is the difference between the observed and calculated transition.

| J' | $K_{a'}$ | $K_{c'}$ | F' | | J | $K_a$ | $K_c$ | F | Observed (MHz) | OMC (MHz) |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 1 | 3 | 4 | ← | 2 | 1 | 2 | 3 | 6312.2657 | -0.0049 |
| 3 | 1 | 3 | 2 | ← | 2 | 1 | 2 | 1 | 6312.2657 | -0.0117 |
| 3 | 0 | 3 | 4 | ← | 2 | 0 | 2 | 3 | 6567.8854 | -0.0013 |
| 3 | 1 | 2 | 4 | ← | 2 | 1 | 1 | 3 | 6938.2031 | -0.0039 |
| 4 | 0 | 4 | 4 | ← | 3 | 0 | 3 | 3 | 8682.4037 | -0.0024 |
| 4 | 0 | 4 | 5 | ← | 3 | 0 | 3 | 4 | 8682.4037 | -0.0029 |
| 4 | 1 | 3 | 3 | ← | 3 | 1 | 2 | 2 | 9228.5603 | 0.0062 |
| 5 | 1 | 5 | 4 | ← | 4 | 1 | 4 | 3 | 10470.9522 | 0.0026 |
| 8 | 1 | 7 | 7 | ← | 7 | 1 | 6 | 6 | 18080.9490 | 0.0082 |
| 8 | 1 | 7 | 9 | ← | 7 | 1 | 6 | 8 | 18080.9490 | -0.0136 |
| 8 | 1 | 7 | 8 | ← | 7 | 1 | 6 | 7 | 18080.9490 | -0.0143 |
| 9 | 1 | 9 | 10 | ← | 8 | 1 | 8 | 9 | 18636.0640 | 0.0041 |
| 9 | 1 | 9 | 8 | ← | 8 | 1 | 8 | 7 | 18636.0640 | 0.0181 |
| 9 | 1 | 9 | 9 | ← | 8 | 1 | 8 | 8 | 18636.0640 | 0.0137 |
| 9 | 0 | 9 | 8 | ← | 8 | 0 | 8 | 7 | 18724.8773 | -0.0177 |
| 10 | 1 | 10 | 9 | ← | 9 | 1 | 9 | 8 | 20653.9944 | 0.0089 |
| 10 | 1 | 10 | 10 | ← | 9 | 1 | 9 | 9 | 20653.9944 | 0.0041 |
| 10 | 1 | 10 | 11 | ← | 9 | 1 | 9 | 10 | 20653.9944 | -0.0025 |
| 10 | 0 | 10 | 11 | ← | 9 | 0 | 9 | 10 | 20711.3929 | 0.0307 |
| 10 | 0 | 10 | 10 | ← | 9 | 0 | 9 | 9 | 20711.3929 | 0.0299 |
| 9 | 2 | 7 | 10 | ← | 8 | 2 | 6 | 9 | 20762.8023 | 0.0077 |
| 10 | 1 | 9 | 11 | ← | 9 | 1 | 8 | 10 | 22209.6025 | 0.0087 |
| 10 | 1 | 9 | 10 | ← | 9 | 1 | 8 | 9 | 22209.6025 | -0.0056 |
| 11 | 1 | 11 | 10 | ← | 10 | 1 | 10 | 9 | 22666.6351 | -0.0131 |
| 11 | 1 | 11 | 11 | ← | 10 | 1 | 10 | 10 | 22666.6351 | -0.0178 |
| 11 | 1 | 11 | 12 | ← | 10 | 1 | 10 | 11 | 22666.6351 | -0.0226 |
| | | | | | | | | | RMS | 11.8 kHz |

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