The Rotational Spectrum and Complete Heavy Atom Structure of the Chiral Molecule Verbenone

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Abstract

As the first step of a two-part chiral tagging experiment, the spectrum and subsequent isotopologue analysis on the heavy atoms of (1S)-(-)-Verbenone is presented. The spectrum has been recorded up to 69 GHz on three spectrometers, one CP-FTMW spectrometer from the University of Virginia functional from 2-8 GHz, a CP-FTMW spectrometer operational in the 6-18 GHz range located at the Missouri University of Science and Technology, and a Stark-modulated spectrometer operational from 48-72 GHz. 1250 transitions have been assigned to the parent and isotopologues for the predominantly *b*-type spectrum. Rotational constants, quartic and sextic centrifugal distortion constants have been determined for the parent species while for the 11 isotopologues only rotational constants have been determined. A Kraitchman analysis has been performed and the resulting coordinates are reported. The

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experimental heavy-atom structure has been compared to the computational structure and is found to be in excellent agreement, showing reliability of the theoretical approaches needed for the future chiral tagging work.

Keywords: Verbenone, CP-FTMW, Rotational Spectroscopy, Chiral, Geometric Structure

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1. Introduction

Chirality is one of the most fundamental aspects of geometric molecular structure, yet one of the hardest aspects of the structure to accurately measure. Recent work in broadband rotational spectroscopy techniques, however, has shown that chirped pulse methods can be harnessed for the qualitative and quantitative distinction of chiral species in racemic mixtures.[1, 2, 3, 4] These, furthermore, can lend some insight into one of the most difficult of chirality measurements, enantiomeric excess (EE).

One recent advancement in accurately determining EE is the process of chiral tagging.[5, 6] Chiral tagging involves using a quantitatively known chiral molecule, binding that molecule through a van der Waals interaction to an unspecified chiral species, and utilizing the conformational differences in the diastereomer complexes. The resulting broadband microwave spectrum can then be used as a way of quantifying EE in both the purely racemic and enantioselective limits. This takes advantage of the high resolution and correct intensity functionality of the technique[7, 8] while avoiding the need for 3-wave mixing techniques and has the potential to be completely theory driven. Proof of principle for this technique, however, involves a thorough structural understanding of the system in question. For these experiments, verbenone was chosen as the structure of unspecified chirality because there had not been a full substitution structure study performed on the molecule.

In addition to being a chiral molecule, verbenone is also a monoterpene. Several similar terpenoids have been studied recently by rotational spectroscopic techniques with splitting in the spectra arising from various motions within the molecules.[9, 10, 11, 12, 1, 13, 14, 15, 16, 17] Our work on verbenone also set out to further understand if any of these internal motions were present in verbenone as well as determine the heavy atom structure of the molecule.

In this work, therefore, we present the first experimental heavy atom structure determination of verbenone using rotational spectroscopy. This structure is compared to the theoretical structure predicted by specialized DFT calculations intended for use in chiral tagging measurements in order to determine the reliability of these methodologies. Furthermore, this structure will lay the groundwork for chiral tagging experiments to be performed with verbenone.

2. Quantum Chemical Calculations

Geometry optimizations were performed with Gaussian09®, Revision E.01[18] at the B3LYP D3BJ level with a def2-TZVP basis set.[19, 20, 21] This particular method and basis set were chosen for reasons that we will briefly highlight, but is based on the work of Grimme and coworkers.[22] First of all, since this molecule was studied as a precursor to complexation with a second chiral molecule as explained above, it is extremely important to have a highly accurate structure while also preserving computational expense. As shown by Grimme and coworkers[22], the typical methods of MP2 and DFT (B3LYP here) have pitfalls in the medium and long-range effects where the structures provided are either too compact (MP2) or too overly repulsive (DFT methods).Grimme's work shows that B2PLYP D3 has the most accurate results but has about the same computational expense as MP2. To get the structure quickly and accurately, the authors have found that B3LYP

D3BJ gives a quality structure for approximately the same computational expense as B3LYP, so this method was chosen. For basis set selection, the best performance in monomers comes with 6-311++G(d,p)[23, 24, 25], but the def2-TZVP[21] basis set gives better complex structures so def2-TZVP was chosen for comparison before and after complexation (chiral tagging). The resulting equilibrium structure is presented in Figure 1 with atomic labels and the quantitative structural parameters are presented in Table 1. The calculated structure predicts dipole moments of 1.00, 4.26, and 0.57 D along the *a*-, *b*-, and *c*-axes, respectively.

Structurally, verbenone is calculated to be a double-ring structure with two methyl groups coming off the carbon labelled atom 6 and one methyl group coming off the carbon labelled atom 1 (see Figure 1). Off of the carbon labelled atom 24, there is an oxygen atom which completes the heavy atom structure. This structure has been quantified in the principal axis system and is presented in Table 2. Verifying the experimental accuracy of this structure is the focus of this work.

3. Experiment

Three spectrometers were used for the acquisition of spectra, a 6-18 GHz CP-FTMW spectrometer located at the Missouri University of Science and Technology (MST), a 2-8 GHz CP-FTMW spectrometer located at the University of Virginia (UVa), and a free jet Stark-modulated spectrometer operational from 48-72 GHz at Monash University. The details of each of these spectrometers have been reported elsewhere.[26, 27, 28, 29] The CP-FTMW setups utilize fast linear frequency sweeps created on an arbitrary waveform generator to create chirped pulses of microwaves on scales $< 10\ \mu$s. These signals are power amplified and broadcast onto the molecules undergoing supersonic expansion in a molecular beam. The instrument at UVa utilized four such beams in one acquisition while the experiment at Missouri S&T used only one. In the Monash setup, solid-state sweep oscillators rather than klystron sources were used to provide improved frequency agility. The radiation source is a YIG-tuned microwave oscillator which produces frequencies in the range of 12-18 GHz, with a frequency quadrupler used to generate the 48-72 GHzl frequency range accessible with the spectrometer. The oscillator is phase-locked to a synthesiser that is referenced to a 5 MHz laboratory frequency standard, allowing frequency measurements accurate to within 1 part in 10^8.The Stark modulation was then provided at 33 kHz between parallel-plate electrodes separated by ≈3.5 cm. Up to 1500 V cm^{-1} electric fields were used to maximize the degree of Stark modulation.

≥93% (1S)-(-)-Verbenone was purchased from Sigma-Aldrich®and was used without further purification. All techniques implemented heating the sample to increase volatility, but did so in different manners. At MST, the sample was heated to 80°C (353 K) approximately 1 m in front of the nozzle in a glass "U"-shaped tube using a Variac and heating tape. Argon gas was bubbled through the heated verbenone at pressures of 6-10 psi and introduced to the instrument through a Parker-Hannifin®Series 9 solenoid valve with 0.8 mm orifice. At UVa, the sample was heated to 65°C (338 K) inside each of the nozzles with a heating apparatus similar to that used in reference [30]. The setup at UVa utilized a neon carrier gas held at approximately 10 psig. 1 million FID averages were collected for each setup. Typical linewidths were ≈60 kHz for the CP-FTMW spectrometers. The Monash setup heated the sample to 80°C (353 K) into a stream of Ar at a pressure of 30 kPa. Sample was introduced through a 350 μm diameter nozzle held at 10°C above the vaporization temperature producing rotational temperatures ∼10 K. The typical linewidths for these spectra were 300-400 kHz. In some instances, linewidths for the Stark-modulated spectrometer were very large to give accurate line centers. In those instances, the attributed uncertainty was set to a value greater than 1 MHz, effectively weighting those transitions in the fit less than the more certain ones.

4. Results and Analysis

The resulting spectra from the CP-FTMW spectrometers are located in Figure 2. Due to the predicted large value of the *b*-component of the dipole moment, assignment was started with *b*-type, R-branch transitions. *a*-type and *c*-type, R-branch transitions were also observed, but with much weaker signal intensity. This was in accordance to their predicted dipole moment values. In addition, a number of *b*-type, Q-branch spectra were observed. Transitions were given an attributed uncertainty of 10 kHz for the CP-FTMW transitions and 10% of the transition linewidth was the attributed uncertainty for the Stark-modulated spectrometer. In total, 633 transitions were assigned to the parent isotopologue between 2-69 GHz. Signal intensity arising from UVa data (≥5000 S:N ratio on some transitions) allowed for the observation of isotopologues consisting of one atom substitution at each heavy atom position in natural abundance, including ^{18}O species. A typical signal intensity profile for these transitions are presented in Figure 3. No splitting arising from internal motion or spin-spin hyperfine due to hydrogen atoms were observed in the spectra, different from other known monoterpenes. This is supported by the CP-FTMW spectral linewidths being on the order of unsplit spectra and only a semi-rigid Hamiltonian being needed for an adequate fit (see below). Assignments were made for these minor isotopologues by using a simple mass substitution into the calculated structure, predicting the rotational constants, and multiplying these constants by the ratio of the experimental parent values to those of the calculated structure.

Spectral fits were performed using Pickett's SPFIT/SPCAT program suite[31] in conjunction with Kisiel's AABS package[32]. The fitted parameters can be found in Table 3. Spectra were fit using a Watson-S Hamiltonian[33] in the I^r representation. In total, 1250 transitions were assigned to 12 different isotopologues with a minimum of 25 transitions assigned for each species. Rotational constants A, B, and C were determined for each isotopologue while all quartic centrifugal distortion constants and four sextic centrifugal distortion constants were determined for the parent. Centrifugal distortion constants for the minor isotopologues were held to the parent values. All microwave RMS values were in good agreement with the attributed measurement uncertainty as evidenced by pure fit RMS values at or below 1.0 for all species. All transition quantum number assignments can be found in the Supplemental Material along with the Pickett input files for the parent species.

Holding the centrifugal distortion constants for the minor isotopologues to the parent value should be addressed. While performing the fits, it was noticed that the size of the centrifugal constants were all very small (especially

D_J) as they typically are with heavy monomer species. This created problems when fitting the minor isotopologues where some fits would cause D_J to be a negative value. Although there is precedent for negative values in D_J, they are rare and inconsistent with the fitted parent value containing over 600 transitions. Although this did not happen with all of the minor isotopologues, for consistency in making accurate structural arguments using these parameters, it was deemed best to hold all centrifugal distortion constants to the values determined for the parent. This, in all cases, had little-to-no effect on the fit RMS which provided more evidence that the other fits with negative D_J values were probably anomalies and that holding the centrifugal distortion terms was the right choice.

5. Discussion

5.1. Experimental Structure and Comparison to Theory

As mentioned in the *Introduction*, verbenone's chiral structure and strong monomer signal makes it a good candidate for chiral tagging measurements. Because of this, verbenone has also been used in subsequent chiral tagging studies with 3-butyn-2-ol to determine an experimental EE of the sample.[6] Typically, chiral information is lost in the Fourier transformation step of the broadband experiment. It has been shown, however, that broadband rotational spectroscopy can be used in a 3-wave mixing scheme to determine EEs utilizing the observed molecular time-domain FID (before Fourier transformation).[1, 2, 3, 4] The problem is that this setup calls for an adjustment to the typical broadband setup. The chiral tagging process eliminates this by taking advantage of the information naturally generated from all

Fourier transform microwave techniques, structure. Since these species are structurally different, their rotational spectra are different. Instead of FID information, this technique takes advantage of the correct intensity profiles of Fourier transformed frequency data to be quantitative.[7, 8] The percentages determined have no theoretical enantiopurity limit because, again, the spectra are a consequence of structural isomers. However, there is a practical limit due to instrument sensitivity from detecting the van der Waals-created diastereomers as the signal must be above the noise floor.

For these initial experiments, a complete experimental structure was needed to further calibrate the tagging procedure and provide a reference point for minor isotopologue species of the monomer. Table 4 presents the experimentally determined Kraitchman[34] coordinates of the heavy-atoms reported with Costain errors.[35] Comparing these values to those provided by theory (Tables 2 and 6) shows that most of the optimized heavy-atom positions are within the uncertainty of the experimental measurement.

In addition to the r_s structure, second moments, inertial defects, and Ray's asymmetry parameter[36] for each isotopologue were determined as both an extra validation of the structure and transition assignments. These are presented in Table 5. Since there was only one substitution structure at each heavy-atom position, these parameters provide a better quantitative structural comparison between isotopologues than rotational constant determination as these structural parameters should be, within reason, relatively invariant to these mass substitutions and can be, if needed, strong evidence of molecular structure where there is no isotopic substitution information.[37] If one of these values, therefore, happened to be well outside agreement with the others, then the outlier fit could be looked at and edited to give a more credible result. Furthermore, second moment values, in conjunction with a quality calculation, can be used as a double-check of atomic labeling of the fits as isotopic substitution of the atoms furthest predicted out-of-planes will have the largest effect on their respective P_{ii} value. The largest changes in these parameters lie with ^{13}C-9, ^{13}C-16, ^{13}C-20, and ^{18}O-25 and are shown by the calculation to be the farthest from the center of mass.

The last thing considered was the accuracy of the quantum chemical calculations from a quantitative perspective. Again, this work utilized a B3LYP D3BJ/def2-TZVP level of theory due to previous success it has had with quickly and accurately determining optimized monomer and dimer structures. It has already been shown in this work that the calculated dipole moments were an accurate reflection of the distribution of observed transitions and there is excellent agreement between the heavy atom positions and the calculated heavy-atom positions. However this work could not, unfortunately, determine substitution at every position in natural abundance. For this, we looked at the percent differences between the calculated and experimental values on the rotational constants. These values were -0.41%, -0.32%, and -0.31% for A, B, and C, respectively, reiterating the excellent agreement between theory and experiment.

In light of all of this evidence, the authors conclude that the r_s experimental structure is so close to the optimized r_e that the two are virtually identical with regards to the heavy-atom positions in the molecule and Figure 1 can be taken as the experimental structure. Being able to calculate structures this accurately at least for the monomer lays some of the groundwork for the theoretically-driven chiral tagging experiments.

5.2. Structural Comparison to other Bicyclic Monoterpenes

All bond lengths and bond angles for verbenone have been determined and are compared to the calculated structure and similar bicyclic monoterpenes nopinone[9], camphor[16], and fenchone[10] in Table 6. Due to possible problems with the r_s structure presented in these previous studies, a r_0 structure of verbenone was undertaken using Kisiel's STRFIT program[38] in order to make direct comparisons. All systems were also put in a similar heavy-atom labelling system. The closest species studied to date is nopinone with the only difference being a missing methyl group and verbenone possessing a double bond between the carbons labelled 3 and 4. This is very apparent with the C_4-C_3 bond length being 1.343(47)Å for verbenone and 1.546(6)Å for nopinone. This double bond is also apparent in the $C_5C_4C_3$ and $C_4C_3C_2$ bond angles which are 117.1(19)° and 118.0(18)°, respectively, very close to the expected 120° from a C-C sp^2 hybridized orbital. This is compared to the same angles in nopinone being 111.3(3)° and 114.1(2)°, much closer to the expected 109.5° from a C-C sp^3 hybridized orbital.

One noticeable difference amongst the family of bicyclic monoterpenes presented is the ring strain upon going from a 1-4 linkage in camphor and fenchone to a 1-5 linkage in verbenone and nopinone. This is very apparent in the $C_1C_6C_5$ bond angle. This angle in camphor and fenchone is approximately 95°. This is already a strained molecular structure from the ideal 109.5°, but only off by 15°. When the 1-5 linkage is made, this angle tigtens considerably to 85-86° for verbenone and nopinone, almost 25° off of ideal. This ring strain seems to be repeated in the $C_5C_7C_1$, $C_7C_1C_6$, and $C_7C_5C_6$

bond angles of verbenone showing that the four membered ring component of the bicyclic monoterpene is even more hindered sterically than those of cyclobutane.

6. Conclusions

The CP-FTMW spectrum of (1S)-(-)-Verbenone has been reported as a first step in a two-part chiral tagging experiment. The transition intensities of the singularly-substituted minor isotopologues of the heavy atoms in the molecule are easily observed in natural abundance allowing for a fully determined heavy-atom structure to be reported for the first time. This structure has been compared to theoretical methods that have been shown to quickly and accurately determine structural parameters, i.e. rotational constants, of midsize molecules ($<$500 amu). The agreement of the experimentally determined heavy atom positions to those of theory is excellent; additionally all theoretical rotational constants are within $<$0.5% error of the experimentally determined values. The authors have concluded that this excellent agreement between experiment and theory is so close that the calculated structure presented in Figure 1 can essentially be considered the experimental structure. The potential for performing chiral analysis of verbenone by attaching a smaller chiral tag molecule, then, is suggested by the high sensitivity of the verbenone monomer spectrum. In the case of the chiral tag measurement, the molecular size is not increased so significantly because verbenone is already a large molecule. As a result, reduction in the transition strength from an increased rotational partition function for the chiral complex may not prohibit sensitive detection of the tagged verbenone.

Previous studies of other monoterpenes, including verbenone, have been shown to have internal motions exhibited by transition splitting in the molecular spectra. No such splitting was observed for this species in any of the measurements made in this work. The combination of high frequency Stark-modulated spectra and high resolution CP-FTMW spectra allowed for both the determination of sextic centrifugal distortion constants and accurate and precise rotational constants for structure. The semirigid Hamiltonian fit used adequately represented the uncertainty attributed to the line centers for all instruments, suggesting no internal rotation unlike that seen in previous monoterpenes.

Structural comparisons to similar bicyclic monoterpenes nopinone, camphor, and fenchone showed that verbenone exhibits very similar characteristics to those systems already studied, but with steric constrictions due to the C-C double bond in the structure. In addition, the four-membered ring in the molecule, like nopinone, exhibits a steric hinderance larger than that of cyclobutane.

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[1] V. A. Shubert, D. Schmitz, C. Medcraft, A. Krin, D. Patterson, J. M. Doyle, M. Schnell, J. Chem. Phys. 142 (2015) 214201.

[2] V. A. Shubert, D. Schmitz, C. Pérez, C. Medcraft, A. Krin, S. R. Domingos, D. Patterson, M. Schnell, J. Phys. Chem. Lett. 7 (2016) 341.

[3] S. Lobsinger, C. Perez, L. Evangelisti, K. K. Lehmann, B. H. Pate, J. Phys. Chem. Lett. 6 (2015) 196.

[4] D. Patterson, M. Schnell, J. M. Doyle, Nature 497 (2013) 475.

[5] N. A. Seifert, C. Pérez, J. L. Neill, B. H. Pate, M. Vallejo-López, A. Lesarri, E. J. Cocinero, F. C. no, Phys. Chem. Chem. Phys. 17 (2015) 18282.

[6] L. Evangelisti, K. J. Mayer, M. S. Holdren, T. Smart, C. West, B. Pate, G. Sedo, F. E. Marshall, G. S. Grubbs II, CHIRAL TAGGING OF VERBENONE WITH 3-BUTYN-2-OL FOR ESTABLISHING ABSOLUTE CONFIGURATION AND DETERMINING ENANTIOMERIC EXCESS, 72nd International Symposium on Molecular Spectroscopy, University of Illinois at Urbana-Champaign, IL, 2017, Accepted, Not Yet Designated a Time.

[7] G. S. Grubbs II, C. T. Dewberry, K. C. Etchison, K. E. Kerr, S. A. Cooke, Rev. Scient. Instrum. 78 (2007) 096106.

[8] G. G. Brown, B. C. Dian, K. O. Douglass, S. M. Geyer, S. T. Shipman, B. H. Pate, Rev. Scient. Instrum. 79 (2008) 053103.

[9] E. M. Neeman, J.-R. Avilés-Moreno, T. R. Huet, Phys. Chem. Chem. Phys. 19 (2017) 13819.

[10] D. Loru, M. Bermúdez, M. E. Sanz, J. Chem. Phys. 145 (2016) 074311.

[11] J. R. A. Moreno, T. R. Huet, J. J. L. González, Struct. Chem. 24 (2013) 1163.

[12] D. Schmitz, V. A. Shubert, B. M. Giuliano, M. Schnell, J. Chem. Phys. 141 (2014) 034304.

[13] D. Schmitz, V. A. Shubert, T. Betz, M. Schnell, Front. Chem. 3 (2015) 15.

[14] H. V. L. Nguyen, H. Mouhib, S. Klahm, W. Stahl, I. Kleiner, Phys. Chem. Chem. Phys. 15 (2013) 10012.

[15] J. R. A. Moreno, F. P. U. na, J. J. L. González, T. R. Huet, Chem. Phys. Lett. 473 (2009) 17.

[16] Z. Kisiel, O. Desyatnyk, E. Bialkowska-Jaworska, L. Pszczółkoski, Phys. Chem. Chem. Phys. 5 (2003) 820.

[17] E. M. Neeman, P. Dréan, T. R. Huet, J. Mol. Spectrosc. 322 (2016) 50.

[18] Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T.

Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Gaussian, Inc., 340 Quinnipiac Street, Building 40, Wallingford, CT, 06492, 2015, copyright © 1994-2015.

[19] P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, J. Phys. Chem 98 (1994) 11623.

[20] S. Grimme, S. Ehrlich, L. Goerigk, J. Comput. Chem. 32 (2011) 1456.

[21] F. Weigend, R. Ahlrichs, Phys. Chem. Chem. Phys. 7 (2005) 3297.

[22] S. Grimme, M. Steinmetz, Phys. Chem. Chem. Phys. 15 (2013) 16031.

[23] R. Krishnan, J. S. Binkley, R. Seeger, J. A. Pople, J. Chem. Phys. 72 (1980) 650.

[24] M. N. Glukhovtsev, A. Pross, M. P. McGrath, L. Radom, J. Chem. Phys. 103 (1995) 1878.

[25] L. A. Curtiss, M. P. McGrath, J.-P. Blandeau, N. E. Davis, R. C. Binning, Jr., L. Radom, J. Chem. Phys. 103 (1995) 6104.

[26] F. E. Marshall, D. J. Gillcrist, T. D. Persinger, S. Jaeger, C. C. Hurley, N. E. Shreve, N. Moon, G. S. Grubbs II, J. Mol. Spectrosc. 328 (2016) 59.

[27] J. L. Neill, S. T. Shipman, L. Alvarez-Valtierra, A. Lesarri, Z. Kisiel, B. H. Pate, J. Mol. Spectrosc. 269 (2011) 21.

[28] C. Pérez, S. Lobsinger, N. A. Seifert, D. P. Zaleski, B. Temelso, G. C. Shields, Z. Kisiel, B. H. Pate, Chem. Phys. Lett. 571 (2013) 1.

[29] D. McNaughton, P. D. Godfrey, J.-U. Grabow, J. Mol. Spectrosc. 274 (2012) 1.

[30] R. D. Suenram, G. Y. Golubiatnikov, I. I. Leonov, J. T. Hougen, J. Ortigoso, I. Kleiner, G. T. Fraser, J. Mol. Spectrosc. 208 (2001) 188.

[31] H. M. Pickett, J. Mol. Spectrosc. 148 (1991) 371.

[32] Z. Kisiel, L. Pszczółkoski, I. R. Medvedev, M. Winnewisser, F. C. D. Lucia, C. E. Herbst, J. Mol. Spectrosc. 233 (2005) 231.

[33] J. K. G. Watson, Vibrational Spectra and Structure 6 (1977) 1.

[34] J. Kraitchman, Am. J. Phys. 21 (1953) 17.

[35] C. C. Costain, Trans. Am. Crystallogr. Assoc. 2 (1966) 157.

[36] W. Gordy, R. L. Cook, Microwave Molecular Spectra; Techniques of Chemistry Vol. XVIII, Wiley, New York, 1984.

[37] R. K. Bohn, J. A. Montgomery, Jr., H. H. Michels, J. A. Fournier, J. Mol. Spectrosc. 325 (2016) 42.

[38] Z. Kisiel, J. Mol. Spectrosc. 218 (2003) 58.

Table 1: Structural parameters and dipole moments from the quantum chemical calculations of verbenone performed at the B3LYP D3BJ/def2-TZVP level.

Parameter	Value
A / MHz	1344
B / MHz	1216
C / MHz	899
D_J / kHz	0.060
D_{JK} / kHz	0.0046
D_K / kHz	-0.042
d_1 / kHz	0.00099
d_2 / kHz	-0.00032
P_{aa} / uÅ^2	301.0
P_{bb} / uÅ^2	261.4
P_{cc} / uÅ^2	114.7
Δ^c / uÅ^2	-229.3
κ^d	0.425
$\lvert\mu_a\rvert$ /D	1.00
$\lvert\mu_b\rvert$ /D	4.26
$\lvert\mu_c\rvert$ /D	0.57

Table 2: Optimized stucture of verbenone in principal axis system.[a]

Atom-Label Number	*a*-coordinate / Å	*b*-coordinate / Å	*c*-coordinate / Å
Carbon-1	1.201	-0.935	-0.030
Carbon-2	1.618	0.321	0.195
Hydrogen-3	2.602	0.565	0.573
Carbon-4	-0.201	-1.111	-0.559
Hydrogen-5	-0.451	-2.157	-0.741
Carbon-6	-1.217	-0.250	0.288
Carbon-7	-0.682	0.952	-0.575
Hydrogen-8	-1.337	1.801	-0.759
Carbon-9	-0.393	-0.076	-1.704
Hydrogen-10	-1.262	-0.272	-2.325
Hydrogen-11	0.473	0.110	-2.336
Carbon-12	2.027	-2.150	0.222
Hydrogen-13	3.023	-1.898	0.584
Hydrogen-14	1.538	-2.793	0.960
Hydrogen-15	2.124	-2.746	-0.691
Carbon-16	-2.669	-0.590	-0.042
Hydrogen-17	-2.940	-1.551	0.403
Hydrogen-18	-3.334	0.167	0.378
Hydrogen-19	-2.867	-0.651	-1.110
Carbon-20	-1.071	-0.190	1.802
Hydrogen-21	-1.728	0.584	2.206
Hydrogen-22	-1.371	-1.141	2.249
Hydrogen-23	-0.058	0.033	2.126
Carbon-24	0.657	1.420	-0.024
Oxygen-25	0.899	2.585	0.225

[a] Optimized structure performed at the B3LYP D3BJ/def2-TZVP level of theory. See text for details.

Table 3: Spectroscopic parameters of all observed isotopologues of verbenone.

Parameter	Parent	^{13}C(1)[a]	^{13}C(2)	^{13}C(4)	^{13}C(6)	^{13}C(7)
A / MHz	1338.4458(1)[b]	1335.6326(4)	1337.9376(3)	1332.9562(3)	1337.9400(3)	1334.2553(2)
B / MHz	1212.0286(1)	1207.6719(3)	1204.3764(3)	1211.1104(3)	1207.6192(3)	1209.6121(2)
C / MHz	895.8775(1)	892.2416(3)	891.5788(3)	893.8687(3)	893.4694(3)	893.7174(2)
D_J / kHz	0.04897(9)	[0.04897][c]	[0.04897]	[0.04897]	[0.04897]	[0.04897]
D_{JK} / kHz	0.0470(1)	[0.0470]	[0.0470]	[0.0470]	[0.0470]	[0.0470]
D_K / kHz	-0.0454(2)	[-0.0454]	[-0.0454]	[-0.0454]	[-0.0454]	[-0.0454]
d_1 / kHz	-0.00893(3)	[-0.00893]	[-0.00893]	[-0.00893]	[-0.00893]	[-0.00893]
d_2 / kHz	0.00368(2)	[0.00368]	[0.00368]	[0.00368]	[0.00368]	[0.00368]
N[d]	633	57	71	73	83	51
RMS[e] / kHz	25.4[f]	10.6	9.3	10.8	8.9	5.5
Parameter	^{13}C(9)	^{13}C(12)	^{13}C(16)	^{13}C(20)	^{13}C(24)	^{18}O(25)
A / MHz	1328.2245(2)	1324.3619(2)	1337.1963(1)	1326.9746(2)	1331.3406(2)	1294.4149(3)
B / MHz	1203.2157(2)	1198.1496(2)	1191.7363(1)	1199.4878(2)	1210.8618(2)	1205.7917(4)
C / MHz	895.6290(1)	882.1853(2)	884.1932(1)	894.0249(1)	892.0564(2)	872.9259(3)
D_J / kHz	[0.04897]	[0.04897]	[0.04897]	[0.04897]	[0.04897]	[0.04897]
D_{JK} / kHz	[0.0470]	[0.0470]	[0.0470]	[0.0470]	[0.0470]	[0.0470]
D_K / kHz	[-0.0454]	[-0.0454]	[-0.0454]	[-0.0454]	[-0.0454]	[-0.0454]
d_1 / kHz	[-0.00893]	[-0.00893]	[-0.00893]	[-0.00893]	[-0.00893]	[-0.00893]
d_2 / kHz	[0.00368]	[0.00368]	[0.00368]	[0.00368]	[0.00368]	[0.00368]
N	44	54	59	50	50	25
RMS / kHz	5.3	6.7	5.1	5.7	5.3	7.2

[a] Number in parentheses in name represents atomic label from Figure 1.

[b] Numbers in parentheses give standard errors (1σ, 67% confidence level) in units of the least significant figure.

[c] Number in brackets have been held to the parent value. See text for details.

[d] Number of observed transitions used in the fit.

[e] RMS is the microwave RMS defined as $\sqrt{\left(\sum\left[(\text{obs}-\text{calc})^2\right]/\text{Nlines}\right)}$.

[f] Using line center accuracy and weighting described in the text, pure RMS was 0.93.

Table 4: Experimentally determined Kraitchman coordinates of each heavy atom in verbenone.

Atom-Label Number	*a*-coordinate / Å	*b*-coordinate / Å	*c*-coordinate / Å
Carbon-1	1.216(1)[a]	-0.910(2)[b]	-0.02(8)
Carbon-2	1.6168(9)	0.338(4)	0.193(8)
Carbon-4	-0.12(1)	-1.120(1)	-0.553(3)
Carbon-6	-1.205(1)	-0.270(6)	0.271(6)
Carbon-7	-0.704(2)	0.933(2)	-0.576(3)
Carbon-9	-0.388(4)	-0.06(2)	-1.7070(9)
Carbon-12	2.0775(7)	-2.1134(7)	0.218(7)
Carbon-16	-2.6572(6)	-0.647(2)	0.00(5)[c]
Carbon-20	-1.056(1)	-0.193(8)	1.8051(8)
Carbon-24	0.618(2)	1.429(1)	-0.02(9)
Oxygen-25	0.841(2)	2.6052(6)	0.216(7)

[a] Number in parentheses represent Costain errors[35] in units of the least significant figure.

[b] Negative sign on coordinates taken from the calculate atom locations.

[c] Kraitchman analysis rendered an imaginary number which has been reported as a value of 0 to the precision of the uncertainty.

Table 5: Second moments, inertial defects, and Ray's asymmetry parameters of all observed isotopologues of verbenone.

Parameter	Parent	^{13}C(1)[a]	^{13}C(2)	^{13}C(4)	^{13}C(6)	^{13}C(7)
P_{aa} / uÅ^2	301.74964(4)[b]	303.2535(1)	304.3625(1)	301.7641(1)	303.1997(1)	302.25493(8)
P_{bb} / uÅ^2	262.36656(4)	263.1615(1)	262.4736(1)	263.6199(1)	262.4369(1)	263.22473(8)
P_{cc} / uÅ^2	115.21990(4)	115.2203(1)	115.2563(1)	115.5216(1)	115.2923(1)	115.54761(8)
Δ^c / uÅ^2	-230.43980(8)	-230.4405(2)	-230.5126(2)	-231.0432(2)	-230.5846(2)	-231.0952(2)
κ^d	0.428711	0.422809	0.401552	0.445004	0.413591	0.434132
Parameter	^{13}C(9)	^{13}C(12)	^{13}C(16)	^{13}C(20)	^{13}C(24)	^{18}O(25)
P_{aa} / uÅ^2	301.90208(6)	306.53471(8)	308.85050(4)	302.88181(6)	302.15116(8)	303.8221(1)
P_{bb} / uÅ^2	262.37063(6)	266.33701(8)	262.72029(4)	262.40335(6)	264.38141(8)	275.1263(1)
P_{cc} / uÅ^2	118.12153(6)	115.26488(8)	115.21899(4)	118.44720(6)	115.22018(8)	115.3042(1)
Δ^c / uÅ^2	-236.2431(1)	-230.5298(2)	-230.43798(8)	-236.8944(1)	-230.4404(2)	-230.6084(3)
κ^d	0.422052	0.429132	0.357797	0.411078	0.451477	0.579476

[a] Number in parentheses in name represents atomic label from Figure 1.

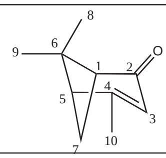
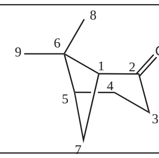
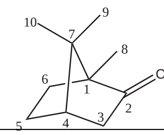
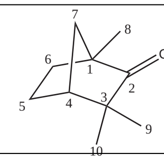
[b] Numbers in parentheses give standard errors

(1σ, 67% confidence level) in units of the least significant figure.

[c] Inertial defect defined as $I_c - I_a - I_b$.

[d] Ray's asymmetry parameter. This value is unitless and is defined as $\kappa = \frac{2B-A-C}{A-C}$.

Table 6: Comparison of verbenone structural parameters to similar bicyclic terpenes.[a]

	Verbenone			Nopinone[9]	Camphor[16]	Fenchone[10]
						
	r_S	r_0	B3LYPD3BJ	r_0	r_0	r_0
$r(C_4\text{-}C_5)$ /Å	1.454(31)[b]	1.510(41)	1.509	1.542(7)	—	—
$r(C_4\text{-}C_{10})$ /Å	1.499(13)	1.496(26)	1.491	—	—	—
$r(C_4\text{-}C_3)$ /Å	1.328(14)	1.343(47)	1.342	1.546(6)	—	—
$r(C_3\text{-}C_2)$ /Å	1.494(13)	1.480(42)	1.476	1.535(7)	1.530(3)	1.535(31)
$r(C_1\text{-}C_2)$ /Å	1.518(33)	1.522(44)	1.522	1.501(11)	1.537(10)	1.526(29)
$r(C_1\text{-}C_7)$ /Å	1.538(13)	1.569(50)	1.554	1.561(6)	—	—
$r(C_1\text{-}C_6)$ /Å	1.5542(69)	1.565(40)	1.573	1.579(11)	1.522(4)	1.541(25)
$r(C_6\text{-}C_8)$ /Å	1.5432(61)	1.528(34)	1.522	1.528(12)	1.542(6)	—
$r(C_6\text{-}C_9)$ /Å	1.524(13)	1.538(24)	1.527	1.535(7)	1.534(5)	—
$r(C_6\text{-}C_5)$ /Å	1.606(11)	1.574(39)	1.578	1.553(9)	1.555(8)	1.552(8)
$r(C_7\text{-}C_5)$ /Å	1.590(14)	1.568(47)	1.555	1.551(10)	—	—
$r(C_2\text{-}O)$ /Å	1.220(17)	1.219(21)	1.216	1.214(4)	1.212(4)	1.214(5)
$\angle(C_{10}C_4C_3)$ /°	123.7(19)	124.1(17)	124.2	—	—	—
$\angle(C_4C_3C_2)$ /°	117.5(12)	118.0(18)	118.0	114.1(2)	—	—
$\angle(C_3C_2O)$ /°	123.6(24)	123.8(28)	123.6	121.4(6)	126.8(1)[c]	125.8(31)
$\angle(C_2C_1C_7)$ /°	107.5(22)	106.8(24)	107.6	108.7(5)	—	—
$\angle(C_2C_1C_6)$ /°	109.5(24)	109.8(22)	109.6	107.7(6)	100.6(3)	—
$\angle(C_1C_6C_8)$ /°	118.16(52)	118.3(29)	118.9	117.6(5)	113.2(4)	—
$\angle(C_1C_6C_5)$ /°	84.97(42)	85.3(18)	84.5	85.9(6)	94.5(4)	95.2(6)
$\angle(C_8C_6C_9)$ /°	106.3(19)	108.1(20)	108.4	108.7(6)	107.5(3)	—
$\angle(C_8C_6C_5)$ /°	118.12(59)	120.1(24)	119.6	119.9(8)	113.7(5)	—
$\angle(C_9C_6C_5)$ /°	114.9(13)	111.9(24)	112.0	112.1(6)	113.7(5)	—
$\angle(C_6C_5C_4)$ /°	110.9(22)	110.1(17)	110.3	111.1(5)	102.6(2)	—
$\angle(C_5C_4C_3)$ /°	118.2(12)	117.1(19)	117.2	111.3(3)	—	—
$\angle(C_5C_4C_{10})$ /°	118.1(11)	118.8(18)	117.2	—	—	—
$\angle(OC_2C_1)$ /°	123.0(14)	122.5(24)	123.0	123.6(6)	126.8(1)[c]	—
$\angle(C_3C_2C_1)$ /°	113.3(12)	113.7(19)	113.4	114.9(4)	—	—
$\angle(C_7C_5C_4)$ /°	109.0(21)	107.2(22)	107.2	108.7(5)	—	—
$\angle(C_7C_5C_6)$ /°	84.59(50)	87.2(22)	87.3	88.3(5)	—	—
$\angle(C_6C_1C_7)$ /°	88.12(62)	87.5(24)	87.5	87.1(5)	—	—
$\angle(C_9C_6C_1)$ /°	113.7(14)	111.7(23)	112.0	111.0(8)	114.1(6)	—
$\angle(C_5C_7C_1)$ /°	86.06(16)	85.3(13)	85.9	86.7(6)	—	—

[a] Atomic labels are made in the schematic graphic for each molecule.

[b] Numbers in parentheses give standard errors (1σ, 67% confidence level) in units of the least significant figure.

[c] $\angle(C_3C_2O) = \angle(OC_2C_1)$ in Ref. [16].

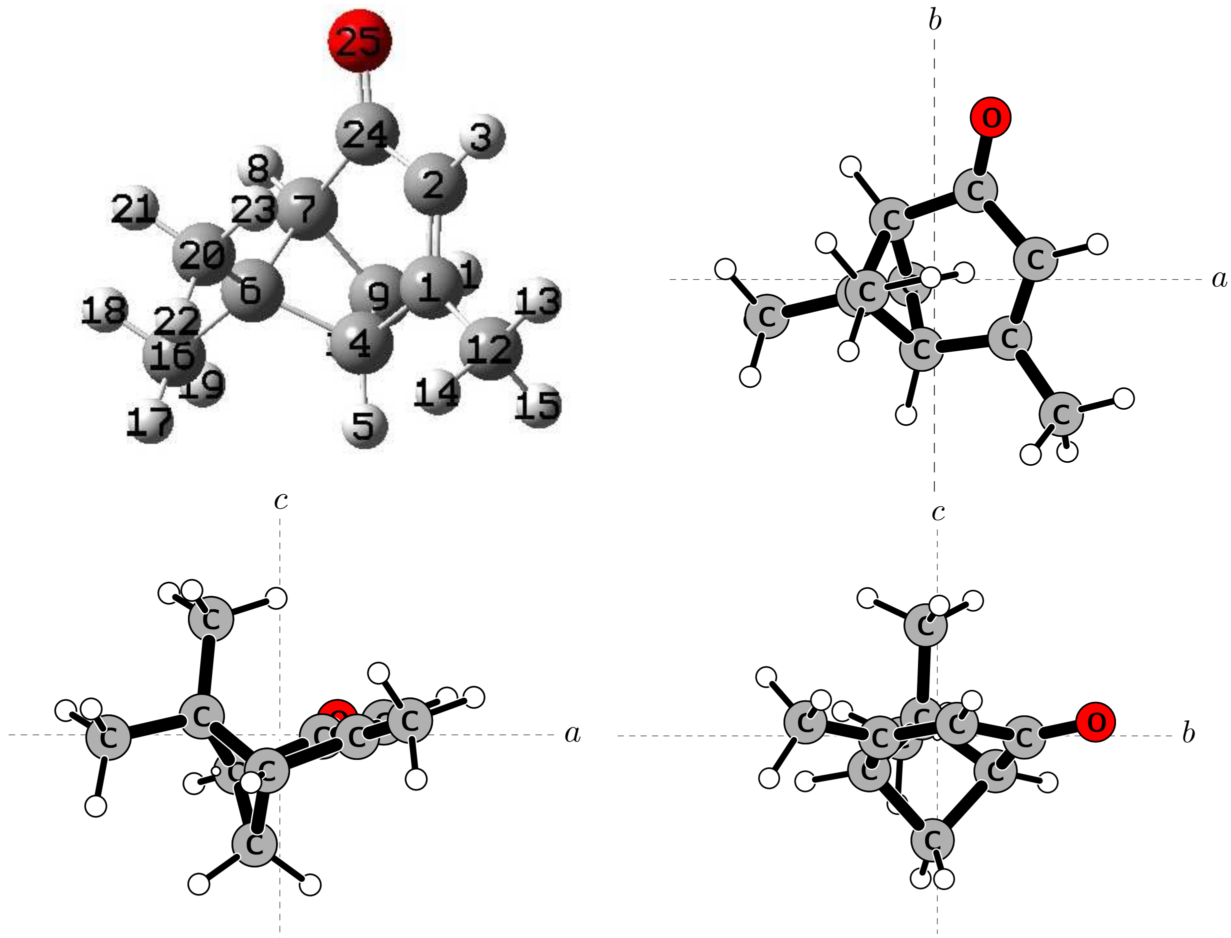


Figure 1: The calculated (see text from details) structure of verbenone showing all heavy-atom labelling and the structure ins the *ab*-, *ac*-, and *bc*-planes.

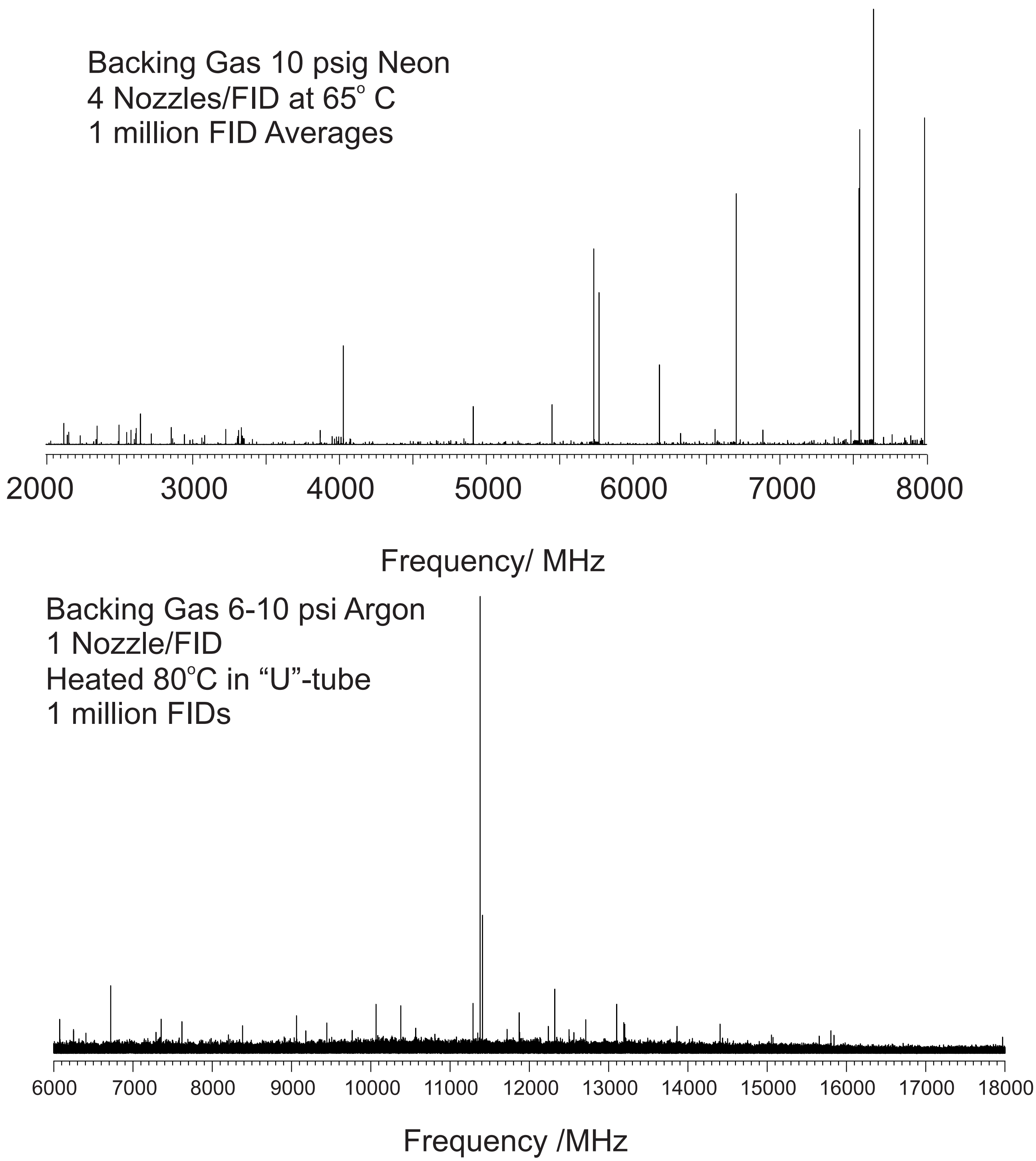


Figure 2: Spectrum of verbenone taken from 2-8 GHz taken at UVa (top) and 6-18 GHz at MST (bottom). Signal-to-noise of the 2-8 GHz spectrum allowed for the observation of all singly-substituted heavy atom isotopologues.

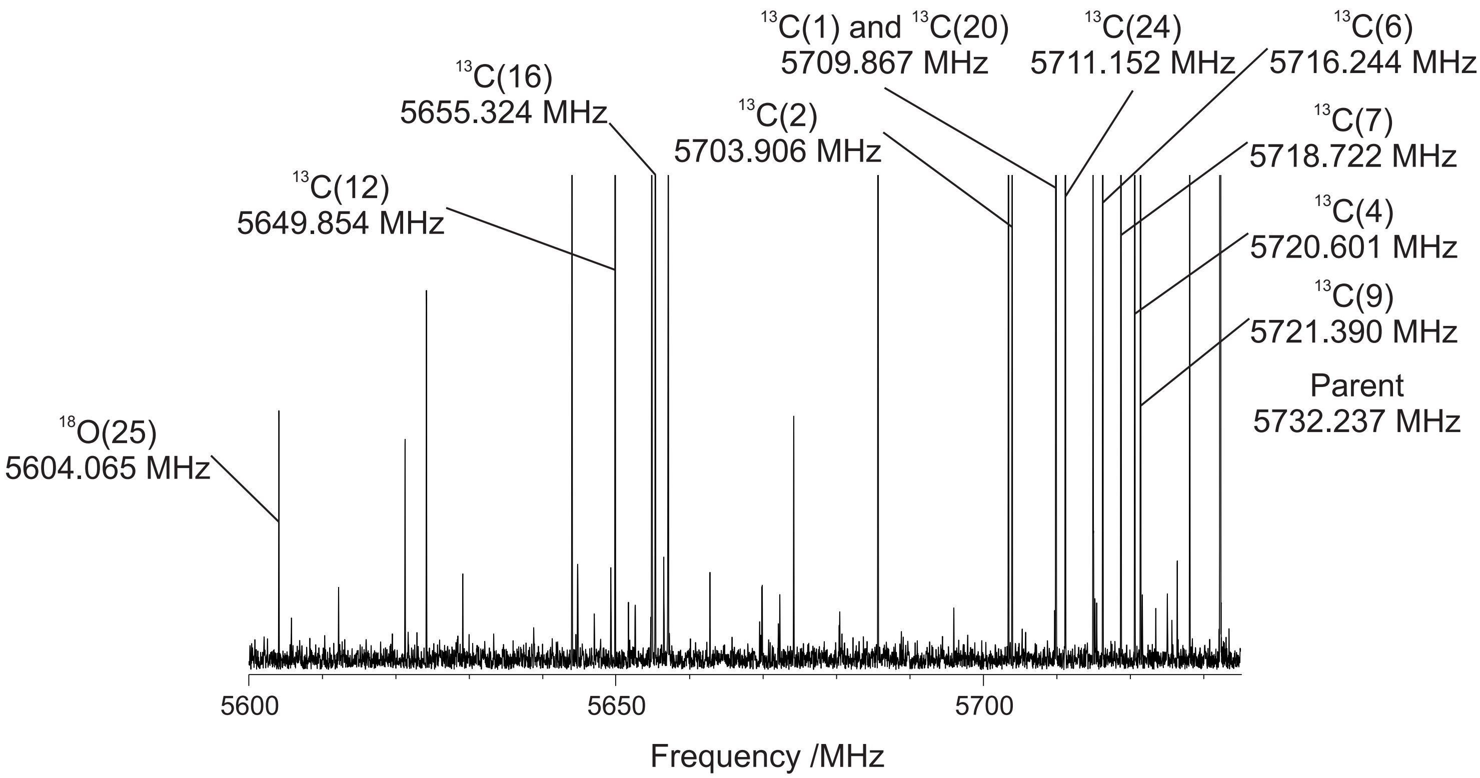


Figure 3: A zoom-in of the UVa spectra from 5600-5735 MHz. The $J'_{K_a,K_c} - J''_{K_a,K_c} = 3_{03} - 2_{12}$ transitions are labeled to show the intensity of the minor isotopologues in natural abundance. Numbers in parentheses represent atomic number labeling from Figure 1. The ^{18}O isotopologue has at least a 10:1 S:N ratio and the ^{13}C species are all too intense at this level to observe their profile maximums.

8. Supplemental Material

All data and calculation outputs for verbenone. Quantum numbers in tables are given as $J'', K_a'', K_c'' \leftarrow J', K_a', K_c'$. Frequency measurements in table are given in MHz.

```
 Parent Verbenone

------------------------------------------------------------------------------------=========
                                              obs         o-c     error     blends     Notes
                                                                          o-c      wt
   / instead of : below denotes (o-c)>3*err
------------------------------------------------------------------------------------=========
   1:  9  7  2   9  6  3                    2033.2573   0.0024  0.010
   2:  5  4  2   5  3  3                    2122.4871   0.0016  0.010
   3:  7  4  3   7  3  4                    2146.4113   0.0022  0.010
   4:  5  5  1   5  4  2                    2155.9200  -0.0035  0.010
   5: 11  8  3  11  7  4                    2159.0846   0.0021  0.010
   6:  1  1  1   0  0  0                    2234.3200  -0.0030  0.010
   7: 12  8  4  12  7  5                    2276.5730   0.0023  0.010
   8:  6  5  2   6  4  3                    2326.2447  -0.0017  0.010
   9:  6  6  0   6  5  1                    2342.3423  -0.0007  0.010
  10:  6  3  3   6  2  4                    2349.0197   0.0024  0.010
  11: 13  9  4  13  8  5                    2365.0783   0.0020  0.010
  12: 11  7  4  11  6  5                    2377.8531   0.0021  0.010
  13:  8  7  1   8  6  2                    2492.8300   0.0026  0.010
  14:  5  2  3   5  1  4                    2498.4277   0.0040  0.010
  15:  6  6  1   6  5  2                    2550.5504  -0.0030  0.010
  16: 10  8  2  10  7  3                    2563.7312   0.0033  0.010
  17:  4  1  3   4  0  4                    2580.0698   0.0210  0.010
  18:  7  6  2   7  5  3                    2602.1811   0.0025  0.010
```

19:	10	6	4	10	5	5	2603.2791	0.0023	0.010
20:	12	9	3	12	8	4	2603.5721	0.0040	0.010
21:	4	2	3	4	1	4	2612.5350	-0.0154	0.010
22:	5	3	3	5	2	4	2615.6031	0.0013	0.010
23:	6	4	3	6	3	4	2644.5286	0.0017	0.010
24:	7	5	3	7	4	4	2718.4978	0.0009	0.010
25:	14	9	5	14	8	6	2779.6549	0.0017	0.010
26:	8	6	3	8	5	4	2854.3711	0.0018	0.010
27:	9	5	4	9	4	5	2863.5682	0.0008	0.010
28:	7	7	0	7	6	1	2874.9252	-0.0017	0.010
29:	8	7	2	8	6	3	2944.0794	0.0015	0.010
30:	7	7	1	7	6	2	2981.7509	-0.0005	0.010
31:	13	8	5	13	7	6	3023.3444	0.0021	0.010
32:	8	4	4	8	4	5	3061.8747	0.0028	0.010
33:	9	7	3	9	6	4	3062.4591	0.0027	0.010
34:	9	8	1	9	7	2	3073.3158	0.0046	0.010
35:	8	4	4	8	3	5	3081.6136	0.0036	0.010
36:	8	6	3	8	4	4	3099.6328	0.0028	0.010
37:	18	12	6	18	11	7	3105.0397	0.0019	0.010
38:	11	9	2	11	8	3	3172.2288	0.0049	0.010
39:	15	11	4	15	10	5	3179.3772	0.0022	0.010
40:	17	12	5	17	11	6	3191.2638	0.0029	0.010
41:	13	10	3	13	9	4	3192.7468	0.0059	0.010
42:	12	7	5	12	7	6	3214.0080	0.0031	0.010
43:	7	3	4	7	3	5	3220.6598	-0.0013	0.010
44:	7	3	4	7	2	5	3225.4411	0.0057	0.010
45:	7	6	2	7	4	3	3266.4018	-0.0050	0.010
46:	19	13	6	19	12	7	3288.1385	0.0006	0.010
47:	6	2	4	6	2	5	3304.5359	-0.0004	0.010
48:	6	2	4	6	1	5	3305.3556	-0.0009	0.010

49:	8	5	4	8	4	5	3307.1350	0.0024	0.010
50:	7	4	4	7	3	5	3312.8022	0.0005	0.010
51:	7	4	4	7	2	5	3317.5807	0.0049	0.010
52:	8	5	4	8	3	5	3326.8736	0.0029	0.010
53:	12	7	5	12	6	6	3331.0440	0.0027	0.010
54:	6	3	4	6	2	5	3331.5925	0.0016	0.010
55:	9	6	4	9	5	5	3332.2641	0.0032	0.010
56:	6	3	4	6	1	5	3332.3988	-0.0122	0.010
57:	9	8	2	9	7	3	3339.2768	0.0021	0.010
58:	10	8	3	10	7	4	3344.2987	0.0033	0.010
59:	5	1	4	5	0	5	3345.5620	0.0050	0.010
60:	9	7	2	9	6	4	3350.6392	0.0067	0.010
61:	5	2	4	5	1	5	3351.1334	0.0014	0.010
62:	8	8	0	8	7	1	3385.7927	0.0064	0.010
63:	10	7	4	10	6	5	3407.4729	0.0022	0.010
64:	16	10	6	16	9	7	3415.2441	0.0015	0.010
65:	8	8	1	8	7	2	3435.5168	0.0004	0.010
66:	20	13	7	20	12	8	3542.2968	0.0092	0.010
67:	11	8	4	11	7	5	3548.8861	0.0029	0.010
68:	3	3	0	3	0	3	3580.8628	-0.0116	0.010
69:	10	7	4	10	5	5	3581.0931	-0.0002	0.010
70:	9	7	3	9	5	4	3595.4992	-0.0004	0.010
71:	11	6	5	11	5	6	3612.7238	0.0016	0.010
72:	10	9	1	10	8	2	3632.5635	0.0044	0.010
73:	11	9	3	11	8	4	3692.7980	0.0037	0.010
74:	20	14	6	20	13	7	3721.5632	0.0039	0.010
75:	15	9	6	15	8	7	3760.1240	0.0018	0.010
76:	22	15	7	22	14	8	3761.7249	-0.0003	0.010
77:	18	13	5	18	12	6	3763.5811	0.0070	0.010
78:	12	9	4	12	8	5	3765.5261	0.0043	0.010

79:	10	9	2	10	8	3	3772.3855	0.0027	0.010
80:	19	12	7	19	11	8	3785.6163	0.0020	0.010
81:	12	10	2	12	9	3	3787.5080	0.0041	0.010
82:	10	5	5	10	5	6	3805.8577	0.0029	0.010
83:	10	5	5	10	4	6	3819.3915	0.0038	0.010
84:	16	12	4	16	11	5	3824.7659	0.0023	0.010
85:	14	11	3	14	10	4	3846.2932	0.0040	0.010
86:	2	0	2	1	1	1	3868.6921	-0.0040	0.010
87:	9	9	0	9	8	1	3879.8552	0.0024	0.010
88:	4	4	0	4	1	3	3896.8597	-0.0109	0.010
89:	2	1	2	1	1	1	3899.6585	-0.0010	0.010
90:	9	9	1	9	8	2	3901.4939	0.0044	0.010
91:	11	8	4	11	6	5	3945.2221	0.0005	0.010
92:	9	4	5	9	4	6	3946.5322	-0.0009	0.010
93:	9	4	5	9	3	6	3950.0955	0.0078	0.010
94:	11	7	5	11	6	6	3966.1163	0.0030	0.010
95:	10	6	5	10	5	6	3979.4811	0.0037	0.010
96:	12	8	5	12	7	6	3989.4245	0.0029	0.010
97:	10	6	5	10	4	6	3993.0152	0.0048	0.010
98:	2	0	2	1	0	1	3995.1097	-0.0036	0.010
99:	11	7	5	11	5	6	4009.0442	-0.0162	0.010
100:	9	5	5	9	4	6	4010.8832	0.0004	0.010
101:	9	5	5	9	3	6	4014.4476	0.0102	0.010
102:	2	1	2	1	0	1	4026.0745	-0.0022	0.010
103:	8	3	5	8	3	6	4026.2518	0.0093	0.010
104:	8	3	5	8	2	6	4026.9790	0.0003	0.010
105:	8	4	5	8	3	6	4045.9895	0.0089	0.010
106:	13	10	4	13	9	5	4057.4130	-0.0061	0.010
107:	13	9	5	13	8	6	4068.5010	0.0017	0.010
108:	7	2	5	7	2	6	4071.5803	0.0026	0.010

109:	7	2	5	7	1	6	4071.6891	0.0037	0.010
110:	7	3	5	7	2	6	4076.3536	0.0018	0.010
111:	7	3	5	7	1	6	4076.4651	0.0055	0.010
112:	8	7	2	8	5	3	4091.1600	-0.0033	0.010
113:	12	10	3	12	9	4	4094.6688	0.0040	0.010
114:	6	1	5	6	0	6	4098.0211	0.0036	0.010
115:	6	2	5	6	1	6	4098.8330	0.0036	0.010
116:	14	8	6	14	7	7	4099.8493	0.0051	0.010
117:	18	11	7	18	10	8	4157.3318	0.0078	0.010
118:	11	10	1	11	9	2	4161.6802	0.0042	0.010
119:	14	10	5	14	9	6	4218.3667	0.0042	0.010
120:	11	10	2	11	9	3	4229.1606	0.0021	0.010
121:	25	17	8	25	16	9	4247.1572	0.0039	0.010
122:	23	16	7	23	15	8	4264.2153	0.0029	0.010
123:	26	17	9	26	16	10	4285.7685	0.0096	0.010
124:	10	8	3	10	6	4	4322.1086	-0.0034	0.010
125:	21	15	6	21	14	7	4357.6637	-0.0136	0.010
126:	10	10	0	10	9	1	4364.2962	0.0140	0.010
127:	27	18	9	27	17	10	4365.4209	0.0059	0.010
128:	13	7	6	13	6	7	4368.7797	0.0063	0.010
129:	13	11	2	13	10	3	4370.5458	0.0083	0.010
130:	10	10	1	10	9	2	4373.2576	0.0054	0.010
131:	14	11	4	14	10	5	4416.1798	0.0052	0.010
132:	5	5	0	5	2	3	4428.2470	-0.0104	0.010
133:	15	11	5	15	10	6	4446.3884	0.0021	0.010
134:	19	14	5	19	13	6	4461.7504	0.0060	0.010
135:	15	12	3	15	11	4	4491.9749	0.0070	0.010
136:	17	13	4	17	12	5	4518.6609	0.0053	0.010
137:	2	1	1	1	1	0	4531.9563	-0.0048	0.010
138:	13	11	3	13	10	4	4534.2763	0.0023	0.010

139:	12	9	4	12	7	5	4540.9393	0.0008	0.010		
140:	12	6	6	12	6	7	4544.0803	0.0151	0.010		
141:	17	10	7	17	9	8	4548.8474	0.0024	0.010		
142:	12	6	6	12	5	7	4552.9880	0.0041	0.010		
143:	14	9	6	14	8	7	4599.8161	0.0036	0.010		
144:	13	8	6	13	7	7	4618.6818	0.0025	0.010		
145:	15	10	6	15	9	7	4623.7986	0.0009	0.010		
146:	12	7	6	12	6	7	4661.1042	0.0025	0.010		
147:	12	11	1	12	10	2	4668.2341	0.0112	0.010		
148:	12	7	6	12	5	7	4670.0256	0.0052	0.010		
149:	11	5	6	11	4	7	4670.6274	0.0020	0.010		
150:	12	11	2	12	10	3	4698.8517	0.0086	0.010		
151:	11	6	6	11	5	7	4711.1037	0.0011	0.010		
152:	11	6	6	11	4	7	4713.5718	-0.0009	0.010		
153:	10	4	6	10	4	7	4744.6245	0.0019	0.010		
154:	10	4	6	10	3	7	4745.1972	0.0042	0.010		
155:	16	12	5	16	11	6	4750.8543	0.0029	0.010		
156:	10	5	6	10	4	7	4758.1583	0.0027	0.010		
157:	10	5	6	10	3	7	4758.7326	0.0067	0.010		
158:	9	3	6	9	2	7	4793.6653	0.0059	0.010		
159:	9	4	6	9	3	7	4797.1152	0.0048	0.010		
160:	9	4	6	9	2	7	4797.2054	-0.0085	0.010		
161:	26	18	8	26	17	9	4820.3724	-0.0062	0.010		
162:	8	2	6	8	1	7	4825.9715	0.0027	0.010		
163:	8	3	6	8	2	7	4826.6943	0.0025	0.010		
164:	15	12	4	15	11	5	4827.6992	0.0042	0.010		
165:	11	11	0	11	10	1	4843.7990	0.0083	0.010		
166:	4	1	4	3	2	1	4843.9413	0.0150	0.010		
167:	11	11	1	11	10	2	4847.3829	0.0057	0.010		
168:	7	2	6	7	1	7	4847.6856	-0.0388	0.010	0.0146	0.50

169:	7	1	6	7	0	7	4847.6856	0.0680	0.010	0.0146 0.50
170:	17	12	6	17	11	7	4870.0173	0.0036	0.010	
171:	16	9	7	16	8	8	4878.6638	0.0029	0.010	
172:	2	2	1	1	1	0	4911.2099	-0.0029	0.010	
173:	14	12	2	14	11	3	4916.4665	-0.0019	0.010	
174:	24	17	7	24	16	8	4962.3460	-0.0028	0.010	
175:	20	12	8	20	11	9	4964.2891	-0.0009	0.010	
176:	2	1	1	1	0	1	4974.5291	-0.0001	0.010	
177:	14	12	3	14	11	4	4997.3280	0.0023	0.010	
178:	16	13	3	16	12	4	5095.5936	0.0068	0.010	
179:	22	16	6	22	15	7	5104.5085	0.0074	0.010	
180:	18	13	6	18	12	7	5111.4931	0.0001	0.010	
181:	15	8	7	15	7	8	5118.3126	0.0046	0.010	
182:	17	13	5	17	12	6	5121.9346	-0.0013	0.010	
183:	5	4	1	5	1	4	5126.3144	0.0093	0.010	
184:	2	2	0	1	1	0	5131.9078	-0.0022	0.010	
185:	13	12	1	13	11	2	5161.3121	0.0115	0.010	
186:	13	12	2	13	11	3	5174.5811	0.0077	0.010	
187:	4	3	1	4	0	4	5183.9454	0.0127	0.010	
188:	6	5	1	6	3	4	5189.9489	0.0062	0.010	
189:	18	14	4	18	13	5	5190.3859	0.0017	0.010	
190:	20	15	5	20	14	6	5191.1158	0.0000	0.010	
191:	6	6	0	6	3	3	5210.3120	-0.0109	0.010	
192:	17	11	7	17	10	8	5213.5640	-0.0026	0.010	
193:	6	5	1	6	2	4	5217.0028	0.0056	0.010	
194:	2	2	1	1	1	1	5227.3627	-0.0011	0.010	
195:	16	10	7	16	9	8	5235.5205	0.0000	0.010	
196:	18	12	7	18	11	8	5240.7106	-0.0021	0.010	
197:	11	9	3	11	7	4	5260.1461	-0.0188	0.010	
198:	16	13	4	16	12	5	5276.0589	-0.0091	0.010	

199:	14	7	7	14	6	8	5279.7714	0.0033	0.010		
200:	15	9	7	15	8	8	5286.8683	-0.0044	0.010		
201:	12	12	0	12	11	1	5320.8720	0.0106	0.010		
202:	12	12	1	12	11	2	5322.2677	0.0122	0.010		
203:	19	13	7	19	12	8	5334.9644	-0.0061	0.010		
204:	14	8	7	14	7	8	5350.2887	-0.0039	0.010		
205:	19	11	8	19	10	9	5352.8088	0.0042	0.010		
206:	13	6	7	13	5	8	5387.2264	-0.0082	0.010		
207:	13	7	7	13	6	8	5413.3792	0.0006	0.010		
208:	19	14	6	19	13	7	5430.1852	-0.0023	0.010		
209:	7	6	1	7	4	4	5431.7384	0.0030	0.010		
210:	15	13	2	15	12	3	5435.2808	0.0079	0.010		
211:	2	2	0	1	1	1	5448.0604	-0.0007	0.010		
212:	12	5	7	12	4	8	5460.6248	0.0044	0.010		
213:	12	6	7	12	5	8	5469.1323	0.0008	0.010		
214:	12	6	7	12	4	8	5469.5578	0.0187	0.010		
215:	15	13	3	15	12	4	5473.0256	0.0111	0.010		
216:	20	14	7	20	13	8	5508.5297	-0.0052	0.010		
217:	11	4	7	11	3	8	5512.4675	0.0052	0.010		
218:	11	5	7	11	4	8	5514.8552	0.0070	0.010		
219:	7	6	1	7	3	4	5523.8801	0.0043	0.010		
220:	18	14	5	18	13	6	5544.7186	-0.0029	0.010		
221:	10	3	7	10	2	8	5549.9192	0.0074	0.010		
222:	10	4	7	10	3	8	5550.4731	0.0045	0.010		
223:	2	2	0	1	0	1	5574.4746	-0.0037	0.010		
224:	9	2	7	9	1	8	5577.1339	0.0618	0.010	0.0108	0.50
225:	9	3	7	9	2	8	5577.1339	-0.0401	0.010	0.0108	0.50
226:	27	19	8	27	18	9	5577.6979	0.0113	0.010		
227:	8	1	7	8	0	8	5596.5048	-0.0035	0.010	-0.0101	0.50
228:	8	2	7	8	1	8	5596.5048	-0.0166	0.010	-0.0101	0.50

229:	14	13	1	14	12	2	5647.0119	-0.0047	0.010
230:	18	10	8	18	9	9	5649.2652	-0.0051	0.010
231:	14	13	2	14	12	3	5652.5851	0.0152	0.010
232:	17	14	3	17	13	4	5656.4747	-0.0087	0.010
233:	3	0	3	2	1	2	5732.2365	-0.0053	0.010
234:	3	1	3	2	1	2	5737.1521	-0.0040	0.010
235:	17	14	4	17	13	5	5747.0236	-0.0058	0.010
236:	3	0	3	2	0	2	5763.2017	-0.0034	0.010
237:	21	15	7	21	14	8	5765.0430	-0.0054	0.010
238:	3	1	3	2	0	2	5768.1164	-0.0030	0.010
239:	20	13	8	20	12	9	5811.3504	-0.0017	0.010
240:	19	15	4	19	14	5	5811.5536	0.0072	0.010
241:	20	15	6	20	14	7	5814.8513	-0.0066	0.010
242:	19	12	8	19	11	9	5833.9881	-0.0047	0.010
243:	21	14	8	21	13	9	5844.0019	-0.0089	0.010
244:	8	7	1	8	5	4	5849.7665	0.0075	0.010
245:	17	9	8	17	8	9	5857.2661	0.0017	0.010
246:	23	17	6	23	16	7	5864.5172	-0.0016	0.010
247:	21	16	5	21	15	6	5884.8166	0.0004	0.010
248:	18	11	8	18	10	9	5892.0687	-0.0053	0.010
249:	16	14	2	16	13	3	5937.4909	-0.0182	0.010
250:	22	15	8	22	14	9	5949.1088	-0.0066	0.010
251:	16	14	3	16	13	4	5954.3771	-0.0104	0.010
252:	17	10	8	17	9	9	5967.1443	-0.0059	0.010
253:	17	10	8	17	8	9	5978.0961	0.0104	0.010
254:	16	8	8	16	7	9	6000.2597	0.0047	0.010
255:	19	15	5	19	14	6	6003.0441	-0.0044	0.010
256:	16	9	8	16	8	9	6045.1115	-0.0134	0.010
257:	8	7	1	8	4	4	6095.0213	0.0016	0.010
258:	22	16	7	22	15	8	6099.1175	0.0004	0.010

259:	15	7	8	15	6	9	6100.7059	-0.0087	0.010		
260:	15	8	8	15	7	9	6117.2259	-0.0073	0.010		
261:	23	16	8	23	15	9	6137.2110	-0.0082	0.010		
262:	14	6	8	14	5	9	6173.9044	0.0102	0.010		
263:	3	1	2	2	2	1	6179.4556	0.0053	0.010		
264:	18	15	3	18	14	4	6186.7491	0.0002	0.010		
265:	13	5	8	13	4	9	6228.8494	0.0080	0.010		
266:	18	15	4	18	14	5	6229.8929	0.0071	0.010		
267:	13	6	8	13	5	9	6230.4362	0.0137	0.010		
268:	21	16	6	21	15	7	6249.8102	-0.0018	0.010		
269:	7	7	0	7	4	3	6252.3799	-0.0137	0.010		
270:	5	1	4	4	4	1	6263.9225	0.0007	0.010		
271:	12	4	8	12	3	9	6270.7851	0.0192	0.010		
272:	12	5	8	12	4	9	6271.1714	0.0094	0.010		
273:	11	3	8	11	3	9	6302.8448	0.0329	0.010	-0.0091	0.50
274:	11	4	8	11	3	9	6302.8448	-0.0511	0.010	-0.0091	0.50
275:	3	2	2	2	2	1	6323.7101	-0.0012	0.010		
276:	10	2	8	10	1	9	6327.0833	0.0013	0.010	-0.0054	0.50
277:	10	3	8	10	2	9	6327.0833	-0.0120	0.010	-0.0054	0.50
278:	9	1	8	9	0	9	6345.1203	-0.0082	0.010		
279:	20	16	4	20	15	5	6385.5654	-0.0073	0.010		
280:	23	15	9	23	14	10	6396.2255	-0.0035	0.010		
281:	20	11	9	20	10	10	6405.2816	-0.0057	0.010		
282:	24	17	8	24	16	9	6409.9975	0.0061	0.010		
283:	22	14	9	22	13	10	6417.2431	0.0059	0.010		
284:	9	8	1	9	6	4	6423.9632	0.0196	0.010		
285:	17	15	2	17	14	3	6430.2708	-0.0053	0.010		
286:	24	16	9	24	15	10	6436.5987	0.0012	0.010		
287:	17	15	3	17	14	4	6437.5642	-0.0084	0.010		
288:	21	13	9	21	12	10	6479.8439	-0.0011	0.010		

289:	23	17	7	23	16	8	6498.1327	-0.0104	0.010
290:	4	1	3	3	3	0	6542.8383	0.0014	0.010
291:	3	1	2	2	1	1	6558.7018	-0.0001	0.010
292:	20	12	9	20	11	10	6564.7059	-0.0136	0.010
293:	4	2	3	3	3	0	6575.9821	0.0003	0.010
294:	19	10	9	19	9	10	6586.3506	-0.0001	0.010
295:	24	14	10	24	13	11	6617.0001	-0.0058	0.010
296:	19	11	9	19	10	10	6656.2181	-0.0116	0.010
297:	9	7	2	9	5	5	6682.8903	-0.0030	0.010
298:	8	6	2	8	3	5	6683.8108	0.0084	0.010
299:	19	16	3	19	15	4	6698.0102	-0.0073	0.010
300:	3	2	2	2	1	1	6702.9618	-0.0012	0.010
301:	18	9	9	18	8	10	6715.8735	-0.0128	0.010
302:	22	17	6	22	16	7	6718.7009	-0.0100	0.010
303:	18	10	9	18	9	10	6743.8994	-0.0104	0.010
304:	15	15	0	15	14	1	6746.5955	0.0007	0.010
305:	15	15	1	15	14	2	6746.6454	-0.0218	0.010
306:	9	7	2	9	4	5	6747.2498	0.0067	0.010
307:	25	18	8	25	17	9	6760.2136	-0.0118	0.010
308:	17	8	9	17	7	10	6811.8840	-0.0133	0.010
309:	7	5	2	7	2	5	6815.7448	0.0112	0.010
310:	17	9	9	17	8	10	6822.1452	-0.0167	0.010
311:	3	2	1	2	2	0	6884.2193	-0.0004	0.010
312:	16	7	9	16	6	10	6885.5335	-0.0108	0.010
313:	5	5	1	5	2	4	6894.0268	0.0159	0.010
314:	23	13	10	23	12	11	6925.4272	0.0065	0.010
315:	21	17	4	21	16	5	6926.3317	-0.0083	0.010
316:	15	6	9	15	5	10	6943.3480	-0.0064	0.010
317:	15	7	9	15	6	10	6944.3567	-0.0156	0.010
318:	15	7	9	15	5	10	6944.4125	-0.0034	0.010

319:	24	18	7	24	17	8	6945.7364	-0.0127	0.010		
320:	9	8	1	9	5	4	6956.9923	0.0054	0.010		
321:	26	17	10	26	16	11	6970.6276	-0.0014	0.010		
322:	21	17	5	21	16	6	6973.3612	-0.0014	0.010		
323:	25	16	10	25	15	11	6987.7847	0.0026	0.010		
324:	27	18	10	27	17	11	7020.7433	-0.0066	0.010		
325:	13	4	9	13	3	10	7025.6058	0.0161	0.010		
326:	13	5	9	13	4	10	7025.6592	0.0087	0.010		
327:	27	19	9	27	18	10	7048.4710	-0.0032	0.010		
328:	24	15	10	24	14	11	7052.7415	-0.0063	0.010		
329:	12	3	9	12	2	10	7054.2462	-0.0049	0.010		
330:	27	16	11	27	15	12	7056.9962	0.0075	0.010		
331/	6	4	2	6	1	5	7059.4889	0.0336	0.010		
332:	10	8	2	10	5	5	7074.3840	-0.0039	0.010		
333:	11	2	9	11	1	10	7076.5379	-0.0112	0.010		
334:	10	2	9	10	1	10	7093.5859	-0.0123	0.010		
335:	23	18	5	23	17	6	7106.2300	-0.0150	0.010		
336:	6	1	5	5	4	2	7133.4303	-0.0193	0.010		
337:	23	14	10	23	13	11	7145.5277	-0.0019	0.010		
338:	22	12	10	22	11	11	7147.1365	0.0010	0.010		
339:	28	19	10	28	18	11	7152.9664	-0.0051	0.010		
340:	26	19	8	26	18	9	7174.0465	-0.0098	0.010		
341:	20	17	3	20	16	4	7198.0757	0.0001	0.010		
342:	20	17	4	20	16	5	7206.8163	-0.0101	0.010		
343:	23	18	6	23	17	7	7207.5782	0.0096	0.010		
344:	16	16	0	16	15	1	7221.0913	0.0157	0.010	0.0027	0.50
345:	16	16	1	16	15	2	7221.0913	-0.0104	0.010	0.0027	0.50
346:	25	19	6	25	18	7	7224.8209	0.0194	0.010		
347:	22	13	10	22	12	11	7249.1125	-0.0081	0.010		
348:	27	20	7	27	19	8	7266.0439	-0.0008	0.010		

349:	21	11	10	21	10	11	7307.7774	-0.0146	0.010
350:	21	12	10	21	11	11	7351.4018	-0.0140	0.010
351:	28	20	9	28	19	10	7415.4075	0.0027	0.010
352:	4	1	3	3	2	1	7423.3273	-0.0044	0.010
353:	25	19	7	25	18	8	7425.4958	-0.0036	0.010
354:	20	10	10	20	9	11	7428.0699	-0.0106	0.010
355:	20	11	10	20	10	11	7445.3230	-0.0115	0.010
356:	22	18	4	22	17	5	7446.2476	-0.0032	0.010
357:	22	18	5	22	17	6	7468.1652	-0.0006	0.010
358:	3	2	1	2	1	1	7484.1676	-0.0011	0.010
359:	5	2	4	4	3	1	7500.5942	-0.0070	0.010
360:	6	6	1	6	3	4	7521.3226	-0.0042	0.010
361:	19	9	10	19	8	11	7521.4489	-0.0104	0.010
362:	19	10	10	19	9	11	7527.7449	-0.0100	0.010
363:	3	1	2	2	0	2	7538.1142	-0.0037	0.010
364:	4	0	4	3	1	3	7538.7456	-0.0026	0.010
365:	4	1	4	3	1	3	7539.3922	0.0007	0.010
366:	4	0	4	3	0	3	7543.6567	-0.0058	0.010
367:	4	1	4	3	0	3	7544.3035	-0.0022	0.010
368:	28	18	11	28	17	12	7547.7223	0.0098	0.010
369:	18	8	10	18	7	11	7595.9624	-0.0163	0.010
370:	18	9	10	18	8	11	7598.0760	-0.0102	0.010
371:	27	17	11	27	16	12	7612.9190	0.0077	0.010
372:	27	20	8	27	19	9	7634.5510	0.0237	0.010
373:	3	3	1	2	2	0	7637.8085	-0.0005	0.010
374:	3	2	2	2	1	2	7651.4105	-0.0051	0.010
375:	17	7	10	17	6	11	7656.3988	-0.0160	0.010
376:	24	19	5	24	18	6	7656.5487	-0.0046	0.010
377:	17	8	10	17	7	11	7657.0406	-0.0158	0.010
378:	25	14	11	25	13	12	7683.7979	0.0118	0.010

379:	17	17	0	17	16	1	7695.3720	0.0063	0.010	0.0017	0.50
380:	17	17	1	17	16	2	7695.3720	-0.0030	0.010	0.0017	0.50
381:	11	9	2	11	6	5	7709.1487	-0.0084	0.010		
382:	26	16	11	26	15	12	7711.7020	0.0034	0.010		
383:	15	5	10	15	4	11	7745.9701	-0.0057	0.010		
384:	3	3	0	2	2	0	7764.7145	0.0000	0.010		
385:	14	4	10	14	3	11	7778.6013	-0.0114	0.010		
386:	13	4	10	13	3	11	7804.8303	-0.0183	0.010		
387:	26	20	6	26	19	7	7820.2041	-0.0134	0.010		
388:	12	2	10	12	1	11	7825.6619	-0.0167	0.010		
389:	25	15	11	25	14	12	7825.8555	0.0005	0.010		
390:	11	1	10	11	0	11	7841.9483	-0.0185	0.010		
391:	3	3	1	2	2	1	7858.5089	0.0024	0.010		
392:	20	18	2	20	17	3	7883.8329	-0.0204	0.010		
393:	6	2	5	5	3	2	7887.0149	0.0092	0.010		
394:	26	20	7	26	19	8	7923.6371	-0.0119	0.010		
395:	24	14	11	24	13	12	7941.7023	-0.0029	0.010		
396:	3	3	0	2	2	1	7985.4113	-0.0006	0.010		
397:	4	1	3	3	2	2	8204.5276	-0.0098	0.010		
398:	4	2	3	3	1	2	8381.9444	0.0009	0.010		
399:	4	3	2	3	2	1	9445.1069	-0.0106	0.010		
400:	5	1	4	4	2	3	10065.6956	0.0061	0.010		
401:	5	2	4	4	1	3	10104.4853	0.0000	0.010		
402:	4	4	1	3	3	0	10377.7460	-0.0035	0.010		
403:	4	4	0	3	3	1	10566.6282	0.0151	0.010		
404:	5	2	3	4	3	2	10575.4514	-0.0208	0.010		
405:	4	3	1	3	2	2	10808.4314	0.0099	0.010		
406:	5	3	3	4	2	2	11079.7736	0.0299	0.010		
407:	6	1	5	5	2	4	11871.5345	-0.0024	0.010		
408:	6	2	5	5	1	4	11877.9956	-0.0125	0.010		

409:	4	3	2	3	0	3	12145.4912	-0.0059	0.010		
410:	5	4	2	4	3	1	12238.6973	0.0087	0.010		
411:	6	2	4	5	3	3	12561.2899	-0.0019	0.010		
412:	6	3	4	5	2	3	12711.1898	0.0145	0.010		
413:	6	3	3	5	4	2	12787.8094	-0.0142	0.010		
414:	5	5	1	4	4	0	13101.6268	0.0013	0.010		
415:	5	5	0	4	4	1	13190.6061	0.0031	0.010		
416:	5	4	1	4	3	2	13203.3618	0.0082	0.010		
417:	7	1	6	6	2	5	13665.1763	0.0051	0.010		
418:	7	2	6	6	1	5	13666.1191	0.0198	0.010		
419:	6	4	3	5	3	2	13863.1261	0.0027	0.010		
420:	5	3	2	4	2	3	14056.6811	-0.0108	0.010		
421:	7	2	5	6	3	4	14405.2667	0.0010	0.010		
422:	7	3	5	6	2	4	14437.0874	-0.0069	0.010		
423:	6	5	2	5	4	1	15054.0840	0.0167	0.010		
424:	7	4	4	6	3	3	15400.8865	0.0078	0.010		
425:	6	5	1	5	4	2	15655.7882	-0.0153	0.010		
426:	6	6	1	5	5	0	15804.2305	-0.0142	0.010		
427:	6	6	0	5	5	1	15842.2509	0.0280	0.010		
428:	7	5	3	6	4	2	16714.2897	-0.0044	0.010		
429:	7	6	2	6	5	1	17853.5466	-0.0276	0.010		
430:	21	13	9	20	12	8	48056.7047	0.0000	0.015		
431:	17	12	6	16	9	7	48106.9421	-0.0117	0.015		
432:	17	11	7	16	8	8	48115.5834	-0.0176	0.016		
433:	22	11	11	21	12	10	48136.1124	-0.0197	0.018		
434:	25	4	21	24	5	20	48159.0535	-0.0084	0.020	-0.0085	0.50
435:	25	5	21	24	4	20	48159.0535	-0.0084	0.020	-0.0085	0.50
436:	22	12	11	21	11	10	48195.1608	0.0016	0.019		
437:	19	14	6	18	13	6	48243.7345	0.0306	0.018		
438:	16	7	10	15	4	11	48245.2208	-0.0956	1.030	-0.0041	0.50

439:	16	6	10	15	5	11	48245.2208	0.0874	1.030	-0.0041	0.50
440:	23	10	14	22	9	13	48352.5872	-0.0326	0.013	-0.0062	0.50
441:	23	9	14	22	10	13	48352.5872	0.0203	0.013	-0.0062	0.50
442:	23	15	8	22	16	7	48414.9779	-0.0143	0.016		
443:	26	3	24	25	2	23	48453.6473	0.0301	0.023	0.0302	0.50
444:	26	2	24	25	3	23	48453.6473	0.0301	0.023	0.0302	0.50
445:	24	8	17	23	7	16	48620.9427	-0.0348	0.023	-0.0349	0.50
446:	24	7	17	23	8	16	48620.9427	-0.0348	0.023	-0.0349	0.50
447:	19	15	5	18	14	4	48655.6116	-0.0777	0.031		
448:	19	15	4	18	14	5	48723.1793	0.0920	1.034		
449:	27	1	27	26	0	26	48749.3435	-0.0425	0.021	-0.0425	0.50
450:	27	0	27	26	1	26	48749.3435	-0.0425	0.021	-0.0425	0.50
451:	22	13	9	21	14	8	48753.5154	-0.0311	0.016		
452:	17	9	8	16	8	9	48777.7734	-0.1007	1.032		
453:	22	12	10	21	13	9	48803.4187	-0.0038	0.017		
454:	17	10	8	16	7	9	48902.3212	0.0319	0.026		
455:	25	6	20	24	5	19	48908.3864	-0.0501	0.019	-0.0501	0.50
456:	25	5	20	24	6	19	48908.3864	-0.0501	0.019	-0.0501	0.50
457:	16	6	11	15	3	12	49069.8870	-0.0150	0.037	-0.0118	0.50
458:	16	5	11	15	4	12	49069.8870	-0.0086	0.037	-0.0118	0.50
459:	19	13	6	18	12	7	49106.0054	-0.0055	0.018		
460:	18	11	7	17	10	8	49221.8058	-0.0209	0.017		
461:	22	13	10	21	12	9	49296.0370	-0.0028	0.017		
462:	20	14	7	19	13	6	49333.5872	-0.0421	0.018		
463:	24	9	16	23	8	15	49376.9417	0.0099	0.024	0.0101	0.50
464:	24	8	16	23	9	15	49376.9417	0.0102	0.024	0.0101	0.50
465:	27	1	26	26	2	25	49497.1242	-0.0508	0.027	-0.0509	0.50
466:	27	2	26	26	1	25	49497.1242	-0.0508	0.027	-0.0509	0.50
467:	25	6	19	24	7	18	49658.8555	-0.0388	0.021	-0.0388	0.50
468:	25	7	19	24	6	18	49658.8555	-0.0388	0.021	-0.0388	0.50

469:	19	17	3	18	16	2	49672.1854	0.0854	1.031	-0.0088	0.50
470:	19	17	2	18	16	3	49672.1854	-0.1030	1.031	-0.0088	0.50
471:	17	13	5	16	10	6	49813.6417	-0.0055	0.014		
472:	16	4	12	15	3	13	49873.7250	-0.0469	0.030	-0.0471	0.50
473:	16	5	12	15	2	13	49873.7250	-0.0471	0.030	-0.0471	0.50
474:	23	11	12	22	12	11	49916.0860	-0.0672	0.024		
475:	23	12	12	22	11	11	49929.9721	0.0379	0.027		
476:	26	4	22	25	5	21	49950.3760	-0.0093	0.019	-0.0094	0.50
477:	26	5	22	25	4	21	49950.3760	-0.0093	0.019	-0.0094	0.50
478:	24	9	15	23	10	14	50137.9872	0.0412	0.019	0.0368	0.50
479:	24	10	15	23	9	14	50137.9872	0.0324	0.019	0.0368	0.50
480:	27	3	25	26	2	24	50245.1176	0.0286	0.027	0.0286	0.50
481:	27	2	25	26	3	24	50245.1176	0.0286	0.027	0.0286	0.50
482:	21	14	8	20	13	7	50358.4286	0.0005	0.015		
483:	28	1	28	27	0	27	50540.9234	0.0127	0.020	0.0128	0.50
484:	28	0	28	27	1	27	50540.9234	0.0127	0.020	0.0128	0.50
485:	19	19	1	18	18	0	50622.8905	0.0272	0.026	0.0272	0.50
486:	19	19	0	18	18	1	50622.8905	0.0272	0.026	0.0272	0.50
487:	20	15	6	19	14	5	50686.7277	-0.0152	0.018		
488:	23	12	11	22	13	10	50690.8357	-0.0149	0.017		
489:	23	13	11	22	12	10	50833.4788	0.0135	0.020		
490:	24	10	14	23	11	13	50907.2702	-0.0203	0.025		
491:	24	11	14	23	10	13	50907.5388	0.0652	0.025		
492:	27	3	24	26	4	23	50993.2584	0.0370	0.026	0.0370	0.50
493:	27	4	24	26	3	23	50993.2584	0.0370	0.026	0.0370	0.50
494/	20	15	5	19	14	6	51005.8500	0.0867	0.024		
495:	18	10	8	17	9	9	51031.6344	-0.0185	0.023		
496:	19	12	7	18	11	8	51058.6190	0.0331	0.016		
497:	25	9	17	24	8	16	51165.8161	0.0343	0.021	0.0344	0.50
498:	25	8	17	24	9	16	51165.8161	0.0344	0.021	0.0344	0.50

499:	22	14	9	21	13	8	51185.3505	0.0163	0.016		
500:	23	13	10	22	14	9	51199.0774	0.0433	0.018		
501:	20	14	6	19	13	7	51244.8692	0.0341	0.016		
502:	18	13	6	17	10	7	51261.7572	0.0212	0.017		
503:	28	2	27	27	1	26	51288.7116	0.0431	0.022	0.0431	0.50
504:	28	1	27	27	2	26	51288.7116	0.0431	0.022	0.0431	0.50
505:	18	11	8	17	8	9	51315.6738	0.0343	0.018		
506:	20	16	5	19	15	4	51357.8999	-0.0540	0.032		
507:	20	16	4	19	15	5	51388.3747	0.0873	0.042		
508:	26	6	20	25	7	19	51449.7205	0.0002	0.025	0.0003	0.50
509:	26	7	20	25	6	19	51449.7205	0.0002	0.025	0.0003	0.50
510:	17	7	11	16	4	12	51547.8972	0.0430	0.108	0.0578	0.50
511:	17	6	11	16	5	12	51547.8972	0.0724	0.108	0.0578	0.50
512:	27	4	23	26	5	22	51741.7199	0.0120	0.031		
513:	20	17	4	19	16	3	51866.6760	-0.0867	1.031		
514:	20	17	3	19	16	4	51868.7094	0.1086	1.025		
515:	25	9	16	24	10	15	51924.6688	0.0357	0.018	0.0350	0.50
516:	25	10	16	24	9	15	51924.6688	0.0343	0.018	0.0350	0.50
517:	28	3	26	27	2	25	52036.5451	0.0006	0.022	0.0006	0.50
518:	28	2	26	27	3	25	52036.5451	0.0006	0.022	0.0006	0.50
519:	24	15	9	23	16	8	52177.9446	-0.0320	0.021		
520:	23	14	10	22	13	9	52184.9060	0.0460	0.020		
521:	26	7	19	25	8	18	52201.3054	-0.0005	0.017	-0.0005	0.50
522:	26	8	19	25	7	18	52201.3054	-0.0005	0.017	-0.0005	0.50
523:	29	1	29	28	0	28	52332.4118	-0.0069	0.019	-0.0069	0.50
524:	29	0	29	28	1	28	52332.4118	-0.0069	0.019	-0.0069	0.50
525:	20	18	3	19	17	2	52349.3617	0.0111	0.022	-0.0242	0.50
526:	20	18	2	19	17	3	52349.3617	-0.0596	0.022	-0.0242	0.50
527:	21	15	7	20	14	6	52401.8799	-0.0373	0.016		
528:	25	11	15	24	10	14	52690.0324	-0.0602	1.017	-0.0441	0.50

529:	25	10	15	24	11	14	52690.0324	-0.0278	1.017	-0.0441	0.50
530:	28	4	25	27	3	24	52784.5906	-0.0327	0.019	-0.0327	0.50
531:	28	3	25	27	4	24	52784.5906	-0.0327	0.019	-0.0327	0.50
532:	20	19	2	19	18	1	52825.5700	-0.0061	0.022	-0.0069	0.50
533:	20	19	1	19	18	2	52825.5700	-0.0076	0.022	-0.0069	0.50
534:	26	9	18	25	8	17	52955.0790	-0.0150	0.018	-0.0151	0.50
535:	26	8	18	25	9	17	52955.0790	-0.0150	0.018	-0.0151	0.50
536:	29	2	28	28	1	27	53080.1564	0.0117	0.020		
537:	27	7	21	26	6	20	53240.6023	-0.0142	0.018		
538:	20	20	0	19	19	1	53299.5242	-0.0022	0.022		
539:	21	16	6	20	15	5	53460.5566	-0.0569	1.000		
540:	25	11	14	24	12	13	53466.4620	0.2514	1.000	-0.0423	0.50
541:	25	12	14	24	11	13	53466.4620	-0.3361	1.000	-0.0423	0.50
542:	28	4	24	27	5	23	53533.0213	-0.0042	0.019	-0.0043	0.50
543:	28	5	24	27	4	23	53533.0213	-0.0042	0.019	-0.0043	0.50
544:	21	15	6	20	14	7	53548.0944	-0.0285	0.017		
545:	22	15	8	21	14	7	53615.6980	-0.0051	0.016		
546:	21	16	5	20	15	6	53618.0838	0.0025	0.017		
547:	26	10	17	25	9	16	53712.2692	0.0031	0.017	0.0033	0.50
548:	26	9	17	25	10	16	53712.2692	0.0033	0.017	0.0033	0.50
549:	19	12	8	18	9	9	53753.0846	0.0116	0.017		
550:	29	3	27	28	2	26	53827.9373	-0.0457	0.021	-0.0458	0.50
551:	29	2	27	28	3	26	53827.9373	-0.0457	0.021	-0.0458	0.50
552:	27	8	20	26	7	19	53991.7002	-0.0434	0.022	-0.0434	0.50
553:	27	7	20	26	8	19	53991.7002	-0.0434	0.022	-0.0434	0.50
554:	18	7	11	17	6	12	54014.2235	0.0449	0.045	-0.0138	0.50
555:	18	8	11	17	5	12	54014.2235	-0.0724	0.045	-0.0138	0.50
556:	21	17	5	20	16	4	54048.3255	-0.0779	0.041		
557:	21	17	4	20	16	5	54061.7184	0.0544	0.042		
558:	30	0	30	29	1	29	54123.9665	0.0567	0.032		

559:	28	5	23	27	6	22	54281.8862	-0.0374	0.022		
560:	26	11	16	25	10	15	54474.6986	-0.0284	0.023		
561:	21	18	3	20	17	4	54545.9417	-0.3623	1.000		
562:	29	3	26	28	4	25	54575.9901	-0.0204	0.019		
563:	21	14	7	20	13	8	54698.9777	-0.0028	0.015		
564:	19	14	6	18	11	7	54711.6305	-0.0062	0.015		
565:	27	8	19	26	9	18	54744.7422	-0.0095	0.017		
566:	30	2	29	29	1	28	54871.6077	0.0046	0.019		
567:	21	19	2	20	18	3	55026.4515	-0.0103	0.034	0.0028	0.50
568:	21	19	3	20	18	2	55026.4515	0.0158	0.034	0.0028	0.50
569:	28	7	22	27	6	21	55031.5719	0.0074	0.023		
570:	25	13	12	24	14	11	55052.7274	-0.0232	0.031		
571:	25	14	12	24	13	11	55141.4072	0.0469	0.025		
572:	20	12	8	19	11	9	55149.9640	0.0123	0.022		
573:	26	11	15	25	12	14	55245.6550	0.0344	0.025	-0.0207	0.50
574:	26	12	15	25	11	14	55245.6550	-0.0757	0.025	-0.0207	0.50
575:	29	4	25	28	5	24	55324.3513	0.0159	0.027		
576:	27	9	18	26	10	17	55500.5870	-0.0065	0.032		
577:	21	20	2	20	19	1	55502.3179	0.0353	0.032		
578:	30	2	28	29	3	27	55619.4142	0.0104	0.020		
579:	28	8	21	27	7	20	55782.2905	-0.0152	0.021	-0.0152	0.50
580:	28	7	21	27	8	20	55782.2905	-0.0152	0.021	-0.0152	0.50
581:	21	21	1	20	20	0	55976.1530	-0.0103	0.024		
582:	29	5	24	28	6	23	56073.1081	-0.0016	0.025		
583:	27	11	17	26	10	16	56260.7684	0.0091	0.039	0.0096	0.50
584:	27	10	17	26	11	16	56260.7684	0.0100	0.039	0.0096	0.50
585/	22	17	5	21	16	6	56265.7296	0.0982	0.027		
586:	30	4	27	29	3	26	56367.4257	0.0439	0.033		
587:	28	9	20	27	8	19	56534.6627	-0.0084	0.027		
588:	29	7	23	28	6	22	56822.5459	-0.0035	0.020	-0.0036	0.50

589:	29	6	23	28	7	22	56822.5459	-0.0035	0.020	-0.0036	0.50
590:	22	19	4	21	18	3	57223.8576	0.1591	1.039	0.0149	0.50
591:	22	19	3	21	18	4	57223.8576	-0.1293	1.039	0.0149	0.50
592:	22	20	2	21	19	3	57703.4235	0.0135	0.022	0.0183	0.50
593:	22	20	3	21	19	2	57703.4235	0.0231	0.022	0.0183	0.50
594:	22	21	1	21	20	2	58178.9971	0.0492	0.032		
595:	30	7	24	29	6	23	58613.5890	0.0288	0.026	0.0288	0.50
596:	30	6	24	29	7	23	58613.5890	0.0288	0.026	0.0288	0.50
597:	22	22	0	21	21	1	58652.7263	-0.0470	0.044	-0.0470	0.50
598:	22	22	1	21	21	0	58652.7263	-0.0470	0.044	-0.0470	0.50
599:	29	10	20	28	9	19	59078.7181	0.0351	0.026		
600:	30	8	23	29	7	22	59363.6729	-0.0166	0.023	-0.0166	0.50
601:	30	7	23	29	8	22	59363.6729	-0.0166	0.023	-0.0166	0.50
602:	23	19	4	22	18	5	59416.7578	0.1205	1.048		
603:	23	20	4	22	19	3	59901.4859	0.0646	0.027	0.0088	0.50
604:	23	20	3	22	19	4	59901.4859	-0.0470	0.027	0.0088	0.50
605:	30	9	22	29	8	21	60115.0784	0.0144	0.027	0.0144	0.50
606:	30	8	22	29	9	21	60115.0784	0.0144	0.027	0.0144	0.50
607:	23	21	2	22	20	3	60380.3181	0.0450	0.044		
608:	23	22	2	22	21	1	60855.5933	0.0200	0.021		
609:	30	9	21	29	10	20	60868.2300	0.0020	0.021		
610:	23	23	0	22	22	1	61329.4365	0.0813	0.044	0.0813	0.50
611:	23	23	1	22	22	0	61329.4365	0.0813	0.044	0.0813	0.50
612:	29	12	17	28	13	16	61365.2769	-0.0276	0.029		
613:	24	20	4	23	19	5	62094.5937	-0.4521	1.029	0.0320	0.50
614:	24	20	5	23	19	4	62094.5937	0.5162	1.029	0.0320	0.50
615:	24	21	3	23	20	4	62578.9254	0.0090	0.042		
616:	24	22	3	23	21	2	63057.0883	0.0303	0.023		
617:	24	23	1	23	22	2	63532.1810	0.0204	0.035		
618:	24	24	1	23	23	0	64005.9332	0.0252	0.028		

```
 619: 25 21  5   24 20  4                     64773.1849   0.2157  1.024   0.0205 0.50
 620: 25 21  4   24 20  5                     64773.1849  -0.1748  1.024   0.0205 0.50
 621: 25 22  3   24 21  4                     65256.1184  -0.0249  0.032  -0.0169 0.50
 622: 25 22  4   24 21  3                     65256.1184  -0.0088  0.032  -0.0169 0.50
 623: 25 23  3   24 22  2                     65733.8129   0.0377  0.028   0.0375 0.50
 624: 25 23  2   24 22  3                     65733.8129   0.0372  0.028   0.0375 0.50
 625: 25 24  2   24 23  1                     66208.7809   0.0710  0.034   0.0710 0.50
 626: 25 24  1   24 23  2                     66208.7809   0.0710  0.034   0.0710 0.50
 627: 26 22  4   25 21  5                     67451.3583  -0.0920  1.044  -0.0144 0.50
 628: 26 22  5   25 21  4                     67451.3583   0.0632  1.044  -0.0144 0.50
 629: 26 23  4   25 22  3                     67933.2416   0.0179  0.032   0.0150 0.50
 630: 26 23  3   25 22  4                     67933.2416   0.0119  0.032   0.0150 0.50
 631: 26 24  3   25 23  2                     68410.4584   0.0306  0.036
 632: 26 25  1   25 24  2                     68885.2382   0.0168  0.041   0.0168 0.50
 633: 26 25  2   25 24  1                     68885.2382   0.0168  0.041   0.0168 0.50
--------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated):

        10000         A  /  /MHz        1338.4457(1)                          1
        20000         B  /  /MHz        1212.0285(1)                          2
        30000         C  /  /MHz         895.8774(1)                          3
          200        DJ  /  /kHz           0.0489(1)                          4
         2000        DK  /  /kHz          -0.0453(2)                          5
         1100       DJK  /  /kHz           0.0469(1)                          6
        40100        d1  /  /kHz          -0.00893(3)                         7
        50000        d2  /  /kHz           0.00367(2)                         8

 MICROWAVE AVG =        0.000378 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.025441 MHz, IR RMS =        0.00000
```

```
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.95372         0.95372

 distinct frequency lines in fit:   567
      distinct parameters of fit:     8

                                   upper state  lower state         overall
     limits of quantum number  1:      1   30       0   29            0   30
     limits of quantum number  2:      0   25       0   24            0   25
     limits of quantum number  3:      0   30       0   29            0   30

                 frequency range:        2033       68885

Standard errors are obtained by muliplying the previous errors by:   0.960520

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

       10000         A  /  /MHz        1338.4458(1)                        1
       20000         B  /  /MHz        1212.0286(1)                        2
       30000         C  /  /MHz         895.8775(1)                        3
         200        DJ  /  /kHz           0.04897(9)                       4
        2000        DK  /  /kHz          -0.0454(2)                        5
        1100       DJK  /  /kHz           0.0470(1)                        6
       40100        d1  /  /kHz          -0.00893(3)                       7
       50000        d2  /  /kHz           0.00368(2)                       8

CORRELATION COEFFICIENTS, C.ij:

          A  /     B  /     C  /     -DJ  /   -DK  /   -DJK  /  d1  /   d2  /
```

```
A  /        1.0000
B  /        0.9115   1.0000
C  /        0.8278   0.8382   1.0000
-DJ  /     -0.8131  -0.8978  -0.8749   1.0000
-DK  /     -0.0246   0.0951   0.0493   0.0065   1.0000
-DJK  /    -0.2198  -0.1676  -0.0553  -0.0137  -0.8309   1.0000
d1  /      -0.4446  -0.5811  -0.2545   0.5277  -0.1371   0.2348   1.0000
d2  /       0.1013   0.0751   0.2741  -0.3039  -0.2435   0.3378  -0.2654   1.0000

 Mean value of |C.ij|, i.ne.j =   0.3717
 Mean value of  C.ij,  i.ne.j =  -0.0660


 No correlations with absolute value greater than 0.9950


 Worst fitted lines (obs-calc/error):

   585:    3.7        494:    3.6        331:    3.4        406:    3.0
   474:   -2.9        427:    2.8        429:   -2.8        455:   -2.6
   491:    2.6        447:   -2.5        500:    2.4        462:   -2.4
   372:    2.4        527:   -2.3        520:    2.3        305:   -2.2
   550:   -2.2         17:    2.1        496:    2.1        501:    2.1
   404:   -2.1        625:    2.1        507:    2.1        392:   -2.0
   503:    2.0        449:   -2.0        478:    2.0        418:    2.0
   515:    2.0        284:    2.0        451:   -1.9        346:    1.9
   552:   -1.9        336:   -1.9        271:    1.9        556:   -1.9
   465:   -1.9        197:   -1.9        571:    1.9        214:    1.9
   505:    1.9        390:   -1.8        610:    1.8        386:   -1.8
   249:   -1.8        467:   -1.8        558:    1.8        437:    1.7
```

```
  530:   -1.7        559:   -1.7

  585/ 22 17  5   21 16  6                    56265.7296   0.0982  0.027
  494/ 20 15  5   19 14  6                    51005.8500   0.0867  0.024
  331/  6  4  2    6  1  5                     7059.4889   0.0336  0.010
  406:  5  3  3    4  2  2                    11079.7736   0.0299  0.010
  474: 23 11 12   22 12 11                    49916.0860  -0.0672  0.024
  427:  6  6  0    5  5  1                    15842.2509   0.0280  0.010
  429:  7  6  2    6  5  1                    17853.5466  -0.0276  0.010
  455: 25  6 20   24  5 19                    48908.3864  -0.0501  0.019  -0.0501 0.50
  491: 24 11 14   23 10 13                    50907.5388   0.0652  0.025
  447: 19 15  5   18 14  4                    48655.6116  -0.0777  0.031
----------------------------------------------------------------


 C13(1)

-----------------------------------------------------------------------------------------=========
                                             obs         o-c     error     blends     Notes
                                                                             o-c      wt
   / instead of : below denotes (o-c)>3*err
-----------------------------------------------------------------------------------------=========
  1:  5  4  2    5  3  3                   2127.6287   0.0036  0.010
  2:  7  4  3    7  3  4                   2136.7148  -0.0083  0.010
  3:  5  5  1    5  4  2                   2168.8235   0.0023  0.010
  4: 12  8  4   12  7  5                   2275.0506   0.0260  0.010
  5:  6  5  2    6  4  3                   2335.3237   0.0051  0.010
  6:  6  3  3    6  2  4                   2341.7459  -0.0092  0.010
  7:  5  2  3    5  1  4                   2494.4831  -0.0008  0.010
  8:  8  7  1    8  6  2                   2522.2904  -0.0269  0.010
```

9:	6	6	1	6	5	2	2567.7971	0.0074	0.010
10:	6	4	3	6	3	4	2645.8203	0.0015	0.010
11:	7	5	3	7	4	4	2722.4631	0.0081	0.010
12:	8	6	3	8	5	4	2862.4119	-0.0007	0.010
13:	8	7	2	8	6	3	2963.1597	0.0184	0.010
14:	8	4	4	8	3	5	3072.1278	-0.0042	0.010
15:	7	3	4	7	2	5	3220.2838	-0.0004	0.010
16:	8	5	4	8	4	5	3306.7734	-0.0039	0.010
17:	7	4	4	7	3	5	3311.5481	-0.0012	0.010
18:	6	3	4	6	2	5	3330.2833	0.0060	0.010
19:	9	6	4	9	5	5	3334.1521	0.0027	0.010
20:	11	8	4	11	7	5	3560.2443	0.0051	0.010
21:	11	9	3	11	8	4	3718.5602	0.0138	0.010
22:	2	0	2	1	1	1	3852.6882	-0.0023	0.010
23:	9	4	5	9	3	6	3943.9809	-0.0020	0.010
24:	11	7	5	11	6	6	3965.3681	0.0016	0.010
25:	10	6	5	10	5	6	3977.1550	0.0154	0.010
26:	9	5	5	9	4	6	4008.2192	-0.0028	0.010
27:	2	1	2	1	0	1	4012.3547	-0.0011	0.010
28:	8	3	5	8	2	6	4023.5296	-0.0169	0.010
29:	7	2	5	7	1	6	4069.6479	-0.0035	0.010
30:	7	3	5	7	2	6	4074.6091	0.0080	0.010
31:	2	1	1	1	1	0	4515.2760	0.0206	0.010
32:	9	4	6	9	3	7	4794.5203	0.0133	0.010
33:	11	11	0	11	10	1	4880.0549	-0.0156	0.010
34:	2	2	1	1	1	0	4899.1381	0.0006	0.010
35:	2	2	0	1	1	1	5433.7406	-0.0015	0.010
36:	3	0	3	2	1	2	5709.8667	-0.0297	0.010
37:	3	1	3	2	1	2	5714.9811	-0.0100	0.010
38:	3	0	3	2	0	2	5741.5957	-0.0055	0.010

```
 39:  3  1  3    2  0  2                          5746.6951  -0.0007  0.010
 40:  3  1  2    2  2  1                          6152.2472   0.0130  0.010
 41: 14  7  8   14  6  9                          6173.5367  -0.0082  0.010
 42:  3  2  2    2  2  1                          6299.7236  -0.0102  0.010
 43:  3  1  2    2  1  1                          6536.1151  -0.0010  0.010
 44:  4  2  3    3  3  0                          6542.1208  -0.0055  0.010
 45:  3  2  2    2  1  1                          6683.6162   0.0002  0.010
 46:  3  2  1    2  2  0                          6857.8681  -0.0005  0.010
 47: 16  7  9   16  6 10                          6878.1472  -0.0224  0.010
 48:  3  2  1    2  1  1                          7460.9321   0.0069  0.010
 49:  4  0  4    3  1  3                          7509.4878   0.0005  0.010
 50:  4  1  4    3  1  3                          7510.1761   0.0138  0.010
 51:  3  1  2    2  0  2                          7514.1254   0.0141  0.010
 52:  4  0  4    3  0  3                          7514.5749  -0.0069  0.010
 53:  4  1  4    3  0  3                          7515.2557  -0.0010  0.010
 54:  3  3  1    2  2  0                          7620.5401   0.0016  0.010
 55:  3  3  0    2  2  0                          7745.6985  -0.0039  0.010
 56:  3  3  1    2  2  1                          7839.7276   0.0146  0.010
 57:  3  3  0    2  2  1                          7964.8764  -0.0005  0.010
--------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated):

        10000         A  /  /MHz         1335.6326(3)                          1
        20000         B  /  /MHz         1207.6719(3)                          2
        30000         C  /  /MHz          892.2416(3)                          3
          200        DJ  /  /kHz          [ 0.048971997]                       4
         2000        DK  /  /kHz          [-0.045366893]                       5
         1100       DJK  /  /kHz          [ 0.046960838]                       6
        40100        d1  /  /kHz          [-0.008933346762]                    7
```

```
       50000        d2  /  /kHz          [ 0.003676407495]                    8

 MICROWAVE AVG =        0.000293 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.010651 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        1.06505         1.06505

  distinct frequency lines in fit:    57
       distinct parameters of fit:     3

                                  upper state  lower state         overall
      limits of quantum number  1:      2   16       1   16           1   16
      limits of quantum number  2:      0   11       0   10           0   11
      limits of quantum number  3:      0    9       0   10           0   10

                 frequency range:        2127         7964

 Standard errors are obtained by muliplying the previous errors by:   1.094235

 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

       10000         A  /  /MHz         1335.6326(4)                         1
       20000         B  /  /MHz         1207.6719(3)                         2
       30000         C  /  /MHz          892.2416(3)                         3
         200        DJ  /  /kHz          [ 0.048971997]                      4
        2000        DK  /  /kHz          [-0.045366893]                      5
        1100       DJK  /  /kHz          [ 0.046960838]                      6
       40100        d1  /  /kHz          [-0.008933346762]                   7
       50000        d2  /  /kHz          [ 0.003676407495]                   8
```

```
 CORRELATION COEFFICIENTS, C.ij:

           A  /      B  /      C  /

A  /       1.0000
B  /       0.8007   1.0000
C  /       0.8000   0.8167   1.0000

 Mean value of |C.ij|, i.ne.j =   0.8058
 Mean value of  C.ij,  i.ne.j =   0.8058


 No correlations with absolute value greater than 0.9950


 Worst fitted lines (obs-calc/error):

    36:   -3.0          8:   -2.7          4:    2.6         47:   -2.2
    31:    2.1         13:    1.8         28:   -1.7         33:   -1.6
    25:    1.5         56:    1.5         51:    1.4         21:    1.4
    50:    1.4         32:    1.3         40:    1.3         42:   -1.0
    37:   -1.0          6:   -0.9          2:   -0.8         41:   -0.8
    11:    0.8         30:    0.8          9:    0.7         52:   -0.7
    48:    0.7         18:    0.6         38:   -0.5         44:   -0.5
     5:    0.5         20:    0.5         14:   -0.4         16:   -0.4
    55:   -0.4          1:    0.4         29:   -0.3         26:   -0.3
    19:    0.3          3:    0.2         22:   -0.2         23:   -0.2
    24:    0.2         54:    0.2         10:    0.1         35:   -0.1
    17:   -0.1         27:   -0.1         43:   -0.1         53:   -0.1
     7:   -0.1         39:   -0.1
```

```
    36:  3  0  3    2  1  2                    5709.8667  -0.0297  0.010
     8:  8  7  1    8  6  2                    2522.2904  -0.0269  0.010
     4: 12  8  4   12  7  5                    2275.0506   0.0260  0.010
    47: 16  7  9   16  6 10                    6878.1472  -0.0224  0.010
    31:  2  1  1    1  1  0                    4515.2760   0.0206  0.010
    13:  8  7  2    8  6  3                    2963.1597   0.0184  0.010
    28:  8  3  5    8  2  6                    4023.5296  -0.0169  0.010
    33: 11 11  0   11 10  1                    4880.0549  -0.0156  0.010
    25: 10  6  5   10  5  6                    3977.1550   0.0154  0.010
    56:  3  3  1    2  2  1                    7839.7276   0.0146  0.010
-----------------------------------------------------

 C13(2)

-------------------------------------------------------------------------------------=========
                                              obs         o-c     error     blends     Notes
                                                                         o-c      wt
    / instead of : below denotes (o-c)>3*err
-------------------------------------------------------------------------------------=========
   1:  7  6  1    7  5  2                    2042.0718   0.0056  0.010
   2:  7  4  3    7  3  4                    2101.9726  -0.0019  0.010
   3:  5  4  2    5  3  3                    2146.5147  -0.0004  0.010
   4:  5  5  1    5  4  2                    2215.5503  -0.0039  0.010
   5:  1  1  1    0  0  0                    2229.5080  -0.0081  0.010
   6:  6  3  3    6  2  4                    2314.8767   0.0000  0.010
   7:  6  5  2    6  4  3                    2368.6165   0.0003  0.010
   8:  5  2  3    5  1  4                    2479.5824  -0.0008  0.010
   9:  4  1  3    4  0  4                    2571.9162   0.0215  0.010
  10:  4  2  3    4  1  4                    2609.9231  -0.0164  0.010
```

11:	5	3	3	5	2	4	2615.1887	-0.0120	0.010
12:	6	6	1	6	5	2	2630.1034	-0.0096	0.010
13:	6	4	3	6	3	4	2650.7347	0.0013	0.010
14:	7	6	2	7	5	3	2666.7480	0.0060	0.010
15:	7	5	3	7	4	4	2737.3985	0.0015	0.010
16:	8	7	2	8	6	3	3032.5828	-0.0020	0.010
17:	8	4	4	8	3	5	3036.3855	-0.0005	0.010
18:	7	3	4	7	2	5	3200.5713	0.0058	0.010
19:	6	2	4	6	1	5	3292.9518	0.0006	0.010
20:	8	5	4	8	4	5	3305.8037	0.0058	0.010
21:	7	4	4	7	3	5	3306.9357	-0.0027	0.010
22:	6	3	4	6	2	5	3325.2623	-0.0034	0.010
23:	5	1	4	5	0	5	3339.1513	0.0034	0.010
24:	9	6	4	9	5	5	3341.8779	0.0016	0.010
25:	5	2	4	5	1	5	3346.0542	-0.0063	0.010
26:	10	7	4	10	6	5	3435.8241	-0.0046	0.010
27:	10	5	5	10	4	6	3767.3202	0.0091	0.010
28:	2	0	2	1	1	1	3844.6489	0.0018	0.010
29:	2	1	2	1	1	1	3879.0942	-0.0171	0.010
30:	9	4	5	9	3	6	3920.4458	0.0079	0.010
31:	2	0	2	1	0	1	3978.2162	0.0081	0.010
32:	9	5	5	9	4	6	3998.3876	0.0019	0.010
33:	12	8	5	12	7	6	4003.5807	0.0105	0.010
34:	8	3	5	8	2	6	4010.2879	-0.0017	0.010
35:	2	1	2	1	0	1	4012.6735	0.0010	0.010
36:	7	2	5	7	1	6	4061.7637	0.0094	0.010
37:	7	3	5	7	2	6	4067.8334	-0.0143	0.010
38:	14	11	3	14	10	4	4101.0327	-0.0066	0.010
39:	12	10	3	12	9	4	4241.6906	0.0223	0.010
40:	12	6	6	12	5	7	4496.9936	0.0006	0.010

41:	14	9	6	14	8	7	4596.9751	0.0248	0.010		
42:	11	5	6	11	4	7	4636.7998	0.0149	0.010		
43:	12	7	6	12	6	7	4640.6395	-0.0074	0.010		
44:	11	6	6	11	5	7	4691.4604	0.0104	0.010		
45:	2	2	1	1	1	0	4905.3879	-0.0015	0.010		
46:	2	2	0	1	1	1	5431.8889	0.0008	0.010		
47:	12	5	7	12	4	8	5434.9383	0.0167	0.010		
48:	3	0	3	2	1	2	5703.9059	-0.0026	0.010		
49:	3	1	3	2	1	2	5709.6932	-0.0010	0.010		
50:	3	0	3	2	0	2	5738.3719	-0.0011	0.010		
51:	3	1	3	2	0	2	5744.1587	0.0000	0.010		
52:	3	1	2	2	2	1	6128.3984	0.0211	0.010		
53:	3	2	2	2	2	1	6287.8644	0.0054	0.010		
54:	9	2	8	9	1	9	6336.7286	-0.0107	0.010	-0.0095	0.50
55:	9	1	8	9	0	9	6336.7286	-0.0083	0.010	-0.0095	0.50
56:	3	1	2	2	1	1	6529.0594	-0.0011	0.010		
57:	3	2	2	2	1	1	6688.5422	-0.0001	0.010		
58:	3	2	1	2	2	0	6837.3409	-0.0061	0.010		
59:	12	3	9	12	2	10	7040.4524	-0.0103	0.010		
60:	10	1	9	10	0	10	7084.4294	-0.0266	0.010		
61:	4	0	4	3	1	3	7503.4988	-0.0010	0.010		
62:	4	1	4	3	1	3	7504.3047	0.0043	0.010		
63:	4	0	4	3	0	3	7509.2691	-0.0164	0.010		
64:	4	1	4	3	0	3	7510.0892	0.0031	0.010		
65:	3	3	1	2	2	0	7632.9290	0.0005	0.010		
66:	15	6	10	15	5	11	7724.6897	-0.0034	0.010		
67:	3	3	0	2	2	0	7751.9544	0.0011	0.010		
68:	13	4	10	13	3	11	7790.5626	-0.0120	0.010	-0.0107	0.50
69:	13	3	10	13	2	11	7790.5626	-0.0094	0.010	-0.0107	0.50
70:	3	3	1	2	2	1	7846.6328	0.0033	0.010		

```
 71:  3  3  0    2  2  1                     7965.6554   0.0012  0.010
-------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated):

        10000         A  /  /MHz        1337.9375(3)                          1
        20000         B  /  /MHz        1204.3764(3)                          2
        30000         C  /  /MHz         891.5787(3)                          3
          200        DJ  /  /kHz         [ 0.048971997]                       4
         2000        DK  /  /kHz         [-0.045366893]                       5
         1100       DJK  /  /kHz         [ 0.046960838]                       6
        40100        d1  /  /kHz         [-0.008933346762]                    7
        50000        d2  /  /kHz         [ 0.003676407495]                    8

 MICROWAVE AVG =        0.000331 MHz, IR AVG =       0.00000
 MICROWAVE RMS =        0.009277 MHz, IR RMS =       0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=       0.92768         0.92768

  distinct frequency lines in fit:    69
       distinct parameters of fit:     3

                                    upper state  lower state        overall
      limits of quantum number  1:      1   15       0   15          0   15
      limits of quantum number  2:      0   11       0   10          0   11
      limits of quantum number  3:      0   10       0   11          0   11

                  frequency range:       2042        7965

 Standard errors are obtained by muliplying the previous errors by:   0.948529

```

```
 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

       10000         A  /  /MHz        1337.9376(3)                       1
       20000         B  /  /MHz        1204.3764(3)                       2
       30000         C  /  /MHz         891.5788(3)                       3
         200        DJ  /  /kHz         [ 0.048971997]                    4
        2000        DK  /  /kHz         [-0.045366893]                    5
        1100       DJK  /  /kHz         [ 0.046960838]                    6
       40100        d1  /  /kHz         [-0.008933346762]                 7
       50000        d2  /  /kHz         [ 0.003676407495]                 8

 CORRELATION COEFFICIENTS, C.ij:

          A  /     B  /     C  /

A  /       1.0000
B  /       0.8658   1.0000
C  /       0.8733   0.9138   1.0000

 Mean value of |C.ij|, i.ne.j =   0.8843
 Mean value of  C.ij,  i.ne.j =   0.8843


 No correlations with absolute value greater than 0.9950


 Worst fitted lines (obs-calc/error):

    60:   -2.7         41:    2.5         39:    2.2          9:    2.1
```

```
   52:   2.1        29:  -1.7        47:   1.7        63:  -1.6
   10:  -1.6        42:   1.5        37:  -1.4        11:  -1.2
   68:  -1.1        33:   1.1        44:   1.0        59:  -1.0
   12:  -1.0        54:  -1.0        36:   0.9        27:   0.9
   31:   0.8         5:  -0.8        30:   0.8        43:  -0.7
   38:  -0.7        25:  -0.6        58:  -0.6        14:   0.6
   18:   0.6        20:   0.6         1:   0.6        53:   0.5
   26:  -0.5        62:   0.4         4:  -0.4        22:  -0.3
   66:  -0.3        23:   0.3        70:   0.3        64:   0.3
   21:  -0.3        48:  -0.3        16:  -0.2        32:   0.2
    2:  -0.2        28:   0.2        34:  -0.2        24:   0.2
   45:  -0.1        15:   0.1

   60: 10  1  9   10  0 10                 7084.4294  -0.0266  0.010
   41: 14  9  6   14  8  7                 4596.9751   0.0248  0.010
   39: 12 10  3   12  9  4                 4241.6906   0.0223  0.010
    9:  4  1  3    4  0  4                 2571.9162   0.0215  0.010
   52:  3  1  2    2  2  1                 6128.3984   0.0211  0.010
   29:  2  1  2    1  1  1                 3879.0942  -0.0171  0.010
   47: 12  5  7   12  4  8                 5434.9383   0.0167  0.010
   63:  4  0  4    3  0  3                 7509.2691  -0.0164  0.010
   10:  4  2  3    4  1  4                 2609.9231  -0.0164  0.010
   42: 11  5  6   11  4  7                 4636.7998   0.0149  0.010
--------------------------------------------------------


 C13(4)

----------------------------------------------------------------------------------------=========
                                              obs          o-c      error     blends     Notes
```

```
                                                                                       o-c      wt
     / instead of : below denotes (o-c)>3*err
-------------------------------------------------------------------------------------------=========
   1:  5  4  2   5  3  3                    2102.7252  -0.0026  0.010
   2:  5  5  1   5  4  2                    2114.6544  -0.0036  0.010
   3:  7  4  3   7  3  4                    2167.1706  -0.0010  0.010
   4:  1  1  1   0  0  0                    2226.8249   0.0002  0.010
   5:  6  6  0   6  5  1                    2274.7252  -0.0283  0.010
   6:  6  5  2   6  4  3                    2295.2575   0.0000  0.010
   7:  6  3  3   6  2  4                    2362.0637   0.0020  0.010
   8:  6  6  1   6  5  2                    2496.2304  -0.0072  0.010
   9:  5  2  3   5  1  4                    2501.9452  -0.0021  0.010
  10:  7  6  2   7  5  3                    2557.3472  -0.0072  0.010
  11:  4  1  3   4  0  4                    2577.3287   0.0235  0.010
  12:  4  2  3   4  1  4                    2606.6694  -0.0263  0.010
  13:  5  3  3   5  2  4                    2608.5939   0.0018  0.010
  14:  6  4  3   6  3  4                    2633.8462   0.0028  0.010
  15:  7  5  3   7  4  4                    2700.5299  -0.0045  0.010
  16:  9  7  3   9  6  4                    3018.1993   0.0042  0.010
  17:  8  4  4   8  3  5                    3098.1925  -0.0013  0.010
  18:  7  3  4   7  2  5                    3230.0056  -0.0170  0.010
  19:  9  8  2   9  7  3                    3263.8238   0.0007  0.010
  20: 10  8  3  10  7  4                    3282.5836   0.0053  0.010
  21:  8  5  4   8  4  5                    3299.1737   0.0047  0.010
  22:  6  2  4   6  1  5                    3302.8722  -0.0015  0.010
  23:  7  4  4   7  3  5                    3307.0426  -0.0101  0.010
  24:  9  6  4   9  5  5                    3318.4289  -0.0066  0.010
  25:  6  3  4   6  2  5                    3325.8603   0.0052  0.010
  26:  5  1  4   5  0  5                    3339.6966   0.0118  0.010
  27/  5  2  4   5  1  5                    3344.5181  -0.0321  0.010
```

28:	11	9	3	11	8	4	3612.7238	-0.0087	0.010
29:	12	10	2	12	9	3	3652.5439	-0.0132	0.010
30:	9	9	1	9	8	2	3810.4545	-0.0019	0.010
31:	10	5	5	10	4	6	3837.0392	0.0246	0.010
32:	2	0	2	1	1	1	3863.8242	0.0014	0.010
33:	11	7	5	11	6	6	3957.8016	-0.0069	0.010
34:	12	8	5	12	7	6	3972.4249	0.0074	0.010
35:	10	6	5	10	5	6	3975.0543	0.0126	0.010
36:	2	0	2	1	0	1	3985.6532	-0.0152	0.010
37:	9	5	5	9	4	6	4006.9881	0.0010	0.010
38:	2	1	2	1	0	1	4014.5607	-0.0001	0.010
39:	8	3	5	8	2	6	4024.8066	0.0076	0.010
40:	13	9	5	13	8	6	4037.1928	0.0056	0.010
41:	7	3	5	7	2	6	4069.6479	-0.0194	0.010
42:	2	1	1	1	1	0	4527.1992	0.0014	0.010
43:	11	5	6	11	4	7	4675.8089	-0.0033	0.010
44:	11	6	6	11	5	7	4709.2745	0.0047	0.010
45:	11	11	0	11	10	1	4730.3080	0.0164	0.010
46/	11	11	1	11	10	2	4734.6134	0.0304	0.010
47:	10	4	6	10	3	7	4743.4316	0.0098	0.010
48:	2	2	1	1	1	0	4892.7292	-0.0061	0.010
49:	2	2	0	1	1	1	5434.2643	-0.0010	0.010
50:	8	2	7	8	1	8	5585.0445	0.0206	0.010
51:	3	0	3	2	1	2	5720.6011	-0.0018	0.010
52:	3	1	3	2	1	2	5725.0369	0.0044	0.010
53:	3	0	3	2	0	2	5749.4915	-0.0038	0.010
54:	3	1	3	2	0	2	5753.9235	-0.0012	0.010
55:	3	1	2	2	2	1	6179.7895	0.0054	0.010
56:	3	2	2	2	2	1	6314.9230	-0.0074	0.010
57:	3	1	2	2	1	1	6545.3232	0.0016	0.010

```
  58:  4  2  3    3  3  0                    6574.3772  -0.0112  0.010
  59:  3  2  2    2  1  1                    6680.4704   0.0023  0.010
  60:  3  2  1    2  2  0                    6880.3683   0.0004  0.010
  61: 12  4  9   12  3 10                    7042.0762  -0.0199  0.010  -0.0158 0.50
  62: 12  3  9   12  2 10                    7042.0762  -0.0115  0.010  -0.0158 0.50
  63:  3  2  1    2  1  1                    7470.1995   0.0058  0.010
  64:  4  0  4    3  1  3                    7522.1012   0.0030  0.010
  65:  4  1  4    3  1  3                    7522.6639   0.0055  0.010
  66:  4  0  4    3  0  3                    7526.5269  -0.0006  0.010
  67:  4  1  4    3  0  3                    7527.0879   0.0002  0.010
  68:  3  3  1    2  2  0                    7607.0140   0.0001  0.010
  69:  3  3  0    2  2  0                    7738.4570   0.0092  0.010
  70: 14  5 10   14  4 11                    7766.4275  -0.0149  0.010
  71: 11  1 10   11  0 11                    7825.3943   0.0009  0.010
  72:  3  3  1    2  2  1                    7831.3017  -0.0004  0.010
  73:  3  3  0    2  2  1                    7962.7385   0.0024  0.010
--------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated):

        10000         A  /  /MHz        1332.9562(3)                        1
        20000         B  /  /MHz        1211.1103(3)                        2
        30000         C  /  /MHz         893.8687(3)                        3
          200        DJ  /  /kHz         [ 0.048971997]                     4
         2000        DK  /  /kHz         [-0.045366893]                     5
         1100       DJK  /  /kHz         [ 0.046960838]                     6
        40100        d1  /  /kHz         [-0.008933346762]                  7
        50000        d2  /  /kHz         [ 0.003676407495]                  8

 MICROWAVE AVG =       -0.000514 MHz, IR AVG =        0.00000
```

```
MICROWAVE RMS =        0.010833 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        1.08325         1.08325

 distinct frequency lines in fit:    72
      distinct parameters of fit:     3

                                   upper state  lower state         overall
     limits of quantum number  1:      1   14       0   14           0   14
     limits of quantum number  2:      0   11       0   10           0   11
     limits of quantum number  3:      0   10       0   11           0   11

                 frequency range:        2102        7962

Standard errors are obtained by muliplying the previous errors by:   1.106548

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

       10000         A  /  /MHz         1332.9562(3)                         1
       20000         B  /  /MHz         1211.1104(3)                         2
       30000         C  /  /MHz          893.8687(3)                         3
         200        DJ  /  /kHz          [ 0.048971997]                      4
        2000        DK  /  /kHz          [-0.045366893]                      5
        1100       DJK  /  /kHz          [ 0.046960838]                      6
       40100        d1  /  /kHz          [-0.008933346762]                   7
       50000        d2  /  /kHz          [ 0.003676407495]                   8

CORRELATION COEFFICIENTS, C.ij:

          A  /     B  /     C  /
```

```
A  /        1.0000
B  /        0.8960   1.0000
C  /        0.8809   0.8801   1.0000

 Mean value of |C.ij|, i.ne.j =   0.8857
 Mean value of  C.ij,  i.ne.j =   0.8857


 No correlations with absolute value greater than 0.9950


 Worst fitted lines (obs-calc/error):

    27:   -3.2         46:    3.0          5:   -2.8         12:   -2.6
    31:    2.5         11:    2.4         50:    2.1         41:   -1.9
    18:   -1.7         45:    1.6         61:   -1.6         36:   -1.5
    70:   -1.5         29:   -1.3         35:    1.3         26:    1.2
    58:   -1.1         23:   -1.0         47:    1.0         69:    0.9
    28:   -0.9         39:    0.8         34:    0.7         56:   -0.7
    10:   -0.7          8:   -0.7         33:   -0.7         24:   -0.7
    48:   -0.6         63:    0.6         40:    0.6         65:    0.5
    55:    0.5         20:    0.5         25:    0.5         44:    0.5
    21:    0.5         15:   -0.4         52:    0.4         16:    0.4
    53:   -0.4          2:   -0.4         43:   -0.3         64:    0.3
    14:    0.3          1:   -0.3         73:    0.2         59:    0.2
     9:   -0.2          7:    0.2

    27/  5  2  4    5  1  5                    3344.5181  -0.0321  0.010
    46/ 11 11  1   11 10  2                    4734.6134   0.0304  0.010
```

```
     5:  6  6  0    6  5  1                    2274.7252  -0.0283  0.010
    12:  4  2  3    4  1  4                    2606.6694  -0.0263  0.010
    31: 10  5  5   10  4  6                    3837.0392   0.0246  0.010
    11:  4  1  3    4  0  4                    2577.3287   0.0235  0.010
    50:  8  2  7    8  1  8                    5585.0445   0.0206  0.010
    41:  7  3  5    7  2  6                    4069.6479  -0.0194  0.010
    18:  7  3  4    7  2  5                    3230.0056  -0.0170  0.010
    45: 11 11  0   11 10  1                    4730.3080   0.0164  0.010
---------------------------------------------------------


 C13(6)

-------------------------------------------------------------------------------------=========
                                              obs         o-c     error     blends     Notes
                                                                          o-c      wt
    / instead of : below denotes (o-c)>3*err
-------------------------------------------------------------------------------------=========
   1:  3  0  3    2  1  2                    5716.2436  -0.0024  0.010
   2:  3  1  3    2  1  2                    5721.6288  -0.0008  0.010
   3:  3  0  3    2  0  2                    5749.1070  -0.0079  0.010
   4:  3  1  3    2  0  2                    5754.4988   0.0003  0.010
   5:  3  1  2    2  2  1                    6150.7034   0.0081  0.010
   6:  3  2  2    2  2  1                    6303.2635   0.0044  0.010
   7:  3  1  2    2  1  1                    6541.6575  -0.0003  0.010
   8:  3  2  2    2  1  1                    6694.2221   0.0004  0.010
   9:  3  2  1    2  2  0                    6857.4072   0.0017  0.010
  10:  4  0  4    3  1  3                    7518.8527   0.0010  0.010
  11:  4  1  4    3  1  3                    7519.5828   0.0041  0.010
  12:  4  0  4    3  0  3                    7524.2321  -0.0032  0.010
```

13:	4	1	4	3	0	3	7524.9658	0.0034	0.010
14:	3	3	1	2	2	0	7633.9485	0.0011	0.010
15:	3	3	0	2	2	1	7973.0662	0.0018	0.010
16:	2	2	1	1	1	0	4907.2877	0.0001	0.010
17:	2	1	2	1	0	1	4018.3471	0.0002	0.010
18:	2	0	2	1	1	1	3855.1570	-0.0001	0.010
19:	1	1	1	0	0	0	2231.4052	-0.0040	0.010
20:	2	2	0	1	1	1	5438.1356	0.0004	0.010
21:	9	7	2	9	6	3	2098.8508	0.0083	0.010
22:	7	4	3	7	3	4	2120.6373	0.0030	0.010
23:	5	4	2	5	3	3	2134.7515	-0.0004	0.010
24:	5	5	1	5	4	2	2188.0120	-0.0050	0.010
25:	6	3	3	6	2	4	2329.1557	0.0031	0.010
26:	11	7	4	11	6	5	2346.1234	0.0217	0.010
27:	6	5	2	6	4	3	2348.5512	0.0037	0.010
28:	6	6	0	6	5	1	2397.7836	0.0068	0.010
29:	5	2	3	5	1	4	2487.0063	0.0029	0.010
30:	4	1	3	4	0	4	2574.4670	0.0189	0.010
31:	6	6	1	6	5	2	2593.5653	0.0002	0.010
32:	4	2	3	4	1	4	2609.9231	-0.0182	0.010
33:	5	3	3	5	2	4	2614.1762	0.0018	0.010
34:	7	6	2	7	5	3	2636.6503	-0.0021	0.010
35:	6	4	3	6	3	4	2646.6693	0.0003	0.010
36:	7	5	3	7	4	4	2727.5313	-0.0031	0.010
37:	9	5	4	9	4	5	2825.3525	-0.0049	0.010
38:	7	7	0	7	6	1	2937.2114	0.0102	0.010
39:	8	7	2	8	6	3	2991.7279	0.0102	0.010
40:	7	7	1	7	6	2	3035.3578	0.0015	0.010
41:	8	4	4	8	3	5	3055.5170	-0.0008	0.010
42:	7	3	4	7	2	5	3210.4705	0.0030	0.010

43:	6	2	4	6	1	5	3297.1299	0.0004	0.010
44:	8	5	4	8	4	5	3304.7524	-0.0047	0.010
45:	7	4	4	7	3	5	3308.0345	0.0035	0.010
46:	6	3	4	6	2	5	3326.6037	-0.0081	0.010
47:	9	6	4	9	5	5	3335.7684	-0.0008	0.010
48:	5	1	4	5	0	5	3340.5647	-0.0011	0.010
49:	5	2	4	5	1	5	3346.8488	-0.0049	0.010
50:	9	8	2	9	7	3	3399.8917	0.0022	0.010
51:	10	7	4	10	6	5	3421.1217	-0.0160	0.010
52:	11	6	5	11	5	6	3566.1112	0.0077	0.010
53:	11	8	4	11	7	5	3576.8667	-0.0200	0.010
54:	10	5	5	10	4	6	3789.4145	-0.0067	0.010
55:	10	9	2	10	8	3	3844.9662	-0.0138	0.010
56:	12	10	2	12	9	3	3899.6593	-0.0224	0.010
57:	9	4	5	9	3	6	3932.2605	0.0113	0.010
58:	10	6	5	10	5	6	3971.6703	-0.0167	0.010
59:	2	0	2	1	0	1	3985.4741	-0.0039	0.010
60:	9	5	5	9	4	6	4002.1421	-0.0013	0.010
61:	8	3	5	8	2	6	4016.1001	-0.0059	0.010
62:	8	4	5	8	3	6	4038.0873	0.0013	0.010
63:	7	3	5	7	2	6	4069.8562	-0.0115	0.010
64:	11	10	2	11	9	3	4312.4880	-0.0077	0.010
65:	13	11	2	13	10	3	4484.6963	0.0195	0.010
66:	15	11	5	15	10	6	4505.8737	0.0077	0.010
67:	2	1	1	1	1	0	4516.3001	-0.0248	0.010
68:	14	9	6	14	8	7	4595.3882	-0.0043	0.010
69:	11	5	6	11	4	7	4650.2073	-0.0066	0.010
70:	11	6	6	11	5	7	4698.1322	0.0030	0.010
71:	10	5	6	10	4	7	4747.0497	0.0119	0.010
72:	9	3	6	9	2	7	4783.9562	0.0120	0.010

```
  73:  9  4  6    9  3  7                     4788.0819   0.0123  0.010
  74: 12 11  2   12 10  3                     4791.8602   0.0145  0.010
  75: 14  7  7   14  6  8                     5245.7854   0.0065  0.010
  76: 12  6  7   12  5  8                     5454.6272  -0.0026  0.010
  77:  8  2  7    8  1  8                     5589.8381   0.0021  0.010   0.0103 0.50
  78:  8  1  7    8  0  8                     5589.8381   0.0184  0.010   0.0103 0.50
  79:  9  1  8    9  0  9                     6337.6883  -0.0171  0.010  -0.0181 0.50
  80:  9  2  8    9  1  9                     6337.6883  -0.0190  0.010  -0.0181 0.50
  81:  4  2  3    3  3  0                     6544.6791   0.0050  0.010
  82:  3  2  1    2  1  1                     7465.0632  -0.0027  0.010
  83:  3  3  0    2  2  0                     7756.3689   0.0024  0.010
--------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated):

        10000         A  /  /MHz        1337.9400(3)                          1
        20000         B  /  /MHz        1207.6191(3)                          2
        30000         C  /  /MHz         893.4694(3)                          3
          200        DJ  /  /kHz         [ 0.048971997]                       4
         2000        DK  /  /kHz         [-0.045366893]                       5
         1100       DJK  /  /kHz         [ 0.046960838]                       6
        40100        d1  /  /kHz         [-0.008933346762]                    7
        50000        d2  /  /kHz         [ 0.003676407495]                    8

 MICROWAVE AVG =       -0.000042 MHz, IR AVG =       0.00000
 MICROWAVE RMS =        0.008882 MHz, IR RMS =       0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=       0.88820         0.88820

  distinct frequency lines in fit:    81
       distinct parameters of fit:     3
```

```
                                  upper state  lower state         overall
      limits of quantum number  1:      1   15       0   15           0   15
      limits of quantum number  2:      0   11       0   10           0   11
      limits of quantum number  3:      0    8       0    9           0    9

                  frequency range:        2098         7973

 Standard errors are obtained by muliplying the previous errors by:   0.905120

 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

        10000         A  /  /MHz         1337.9400(3)                    1
        20000         B  /  /MHz         1207.6192(3)                    2
        30000         C  /  /MHz          893.4694(3)                    3
          200        DJ  /  /kHz          [ 0.048971997]                 4
         2000        DK  /  /kHz          [-0.045366893]                 5
         1100       DJK  /  /kHz          [ 0.046960838]                 6
        40100        d1  /  /kHz          [-0.008933346762]              7
        50000        d2  /  /kHz          [ 0.003676407495]              8

 CORRELATION COEFFICIENTS, C.ij:

           A  /     B  /     C  /

A  /        1.0000
B  /        0.9291   1.0000
C  /        0.8935   0.9054   1.0000
```

```
Mean value of |C.ij|, i.ne.j =   0.9094
Mean value of  C.ij,  i.ne.j =   0.9094


No correlations with absolute value greater than 0.9950


Worst fitted lines (obs-calc/error):

   67:   -2.5         56:   -2.2         26:    2.2         53:   -2.0
   65:    1.9         30:    1.9         32:   -1.8         79:   -1.8
   58:   -1.7         51:   -1.6         74:    1.4         55:   -1.4
   73:    1.2         72:    1.2         71:    1.2         63:   -1.1
   57:    1.1         77:    1.0         38:    1.0         39:    1.0
   21:    0.8         46:   -0.8          5:    0.8          3:   -0.8
   52:    0.8         66:    0.8         64:   -0.8         28:    0.7
   54:   -0.7         69:   -0.7         75:    0.6         61:   -0.6
   81:    0.5         24:   -0.5         37:   -0.5         49:   -0.5
   44:   -0.5          6:    0.4         68:   -0.4         11:    0.4
   19:   -0.4         59:   -0.4         27:    0.4         45:    0.3
   13:    0.3         12:   -0.3         25:    0.3         36:   -0.3
   42:    0.3         22:    0.3

   67:  2  1  1    1  1  0                     4516.3001  -0.0248  0.010
   56: 12 10  2   12  9  3                     3899.6593  -0.0224  0.010
   26: 11  7  4   11  6  5                     2346.1234   0.0217  0.010
   53: 11  8  4   11  7  5                     3576.8667  -0.0200  0.010
   65: 13 11  2   13 10  3                     4484.6963   0.0195  0.010
   30:  4  1  3    4  0  4                     2574.4670   0.0189  0.010
   32:  4  2  3    4  1  4                     2609.9231  -0.0182  0.010
```

```
    79:  9  1  8    9  0  9                    6337.6883  -0.0171  0.010  -0.0181 0.50
    58: 10  6  5   10  5  6                    3971.6703  -0.0167  0.010
    51: 10  7  4   10  6  5                    3421.1217  -0.0160  0.010
---------------------------------------------------------------


C13(7)

-------------------------------------------------------------------------------------=========
                                              obs        o-c     error     blends     Notes
                                                                          o-c      wt
    / instead of : below denotes (o-c)>3*err
-------------------------------------------------------------------------------------=========
   1:  5  4  2   5  3  3                    2111.6956   0.0035  0.010
   2:  5  5  1   5  4  2                    2137.9098  -0.0088  0.010
   3:  7  4  3   7  3  4                    2149.0879  -0.0005  0.010
   4:  1  1  1   0  0  0                    2227.9716  -0.0008  0.010
   5:  6  5  2   6  4  3                    2311.2941   0.0044  0.010
   6:  6  6  0   6  5  1                    2315.2779  -0.0074  0.010
   7:  6  3  3   6  2  4                    2348.8088   0.0015  0.010
   8:  5  2  3   5  1  4                    2494.7496   0.0048  0.010
   9:  6  6  1   6  5  2                    2527.4220  -0.0106  0.010
  10:  7  6  2   7  5  3                    2582.0651   0.0073  0.010
  11:  5  3  3   5  2  4                    2608.1217   0.0014  0.010
  12:  6  4  3   6  3  4                    2635.7361  -0.0007  0.010
  13:  7  5  3   7  4  4                    2707.0936  -0.0029  0.010
  14:  8  6  3   8  5  4                    2838.8849  -0.0002  0.010
  15:  9  5  4   9  4  5                    2868.2573  -0.0154  0.010
  16:  8  7  2   8  6  3                    2918.2078   0.0011  0.010
  17:  8  4  4   8  3  5                    3081.2244   0.0025  0.010
```

18:	8	5	4	8	4	5	3297.9382	-0.0024	0.010
19:	6	2	4	6	1	5	3298.0832	0.0004	0.010
20:	7	4	4	7	3	5	3304.3728	-0.0009	0.010
21:	9	8	2	9	7	3	3307.5306	0.0046	0.010
22:	9	6	4	9	5	5	3321.0125	0.0052	0.010
23:	6	3	4	6	2	5	3323.1497	0.0027	0.010
24:	5	2	4	5	1	5	3342.3581	-0.0130	0.010
25:	2	0	2	1	1	1	3860.5571	-0.0014	0.010
26:	9	4	5	9	3	6	3944.1167	0.0003	0.010
27:	2	0	2	1	0	1	3985.1979	-0.0038	0.010
28:	9	5	5	9	4	6	4001.7114	-0.0013	0.010
29:	2	1	2	1	0	1	4015.4058	-0.0003	0.010
30:	2	1	1	1	1	0	4522.5606	0.0088	0.010
31:	9	4	6	9	3	7	4785.5930	0.0096	0.010
32:	2	2	1	1	1	0	4896.4807	-0.0005	0.010
33:	2	2	0	1	1	1	5433.8347	0.0027	0.010
34:	3	0	3	2	1	2	5718.7225	-0.0034	0.010
35:	3	1	3	2	1	2	5723.4643	-0.0009	0.010
36:	3	0	3	2	0	2	5748.9238	-0.0065	0.010
37:	3	1	3	2	0	2	5753.6695	-0.0002	0.010
38:	3	1	2	2	2	1	6169.0755	0.0059	0.010
39:	3	1	2	2	1	1	6543.0035	0.0044	0.010
40:	3	2	2	2	1	1	6683.9116	0.0001	0.010
41:	3	2	1	2	2	0	6871.0323	-0.0032	0.010
42:	3	2	1	2	1	1	7466.4214	0.0002	0.010
43:	4	0	4	3	1	3	7520.5484	0.0001	0.010
44:	3	1	2	2	0	2	7520.8734	-0.0133	0.010
45:	4	1	4	3	1	3	7521.1636	0.0020	0.010
46:	4	0	4	3	0	3	7525.2820	-0.0055	0.010
47:	4	1	4	3	0	3	7525.9014	0.0005	0.010

```
  48:  3  3  1    2  2  0                     7614.1575   0.0018  0.010
  49:  3  2  2    2  1  2                     7631.6040   0.0092  0.010
  50:  3  3  0    2  2  0                     7742.3104   0.0065  0.010
  51:  3  3  0    2  2  1                     7963.7597  -0.0003  0.010
--------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated):

      10000         A  /  /MHz         1334.2552(4)                           1
      20000         B  /  /MHz         1209.6121(3)                           2
      30000         C  /  /MHz          893.7174(3)                           3
        200        DJ  /  /kHz          [ 0.048971997]                        4
       2000        DK  /  /kHz          [-0.045366893]                        5
       1100       DJK  /  /kHz          [ 0.046960838]                        6
      40100        d1  /  /kHz          [-0.008933346762]                     7
      50000        d2  /  /kHz          [ 0.003676407495]                     8

 MICROWAVE AVG =       -0.000253 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.005458 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.54579         0.54579

  distinct frequency lines in fit:    51
       distinct parameters of fit:     3

                                    upper state  lower state        overall
      limits of quantum number  1:      1    9      0    9          0    9
      limits of quantum number  2:      0    8      0    7          0    8
      limits of quantum number  3:      0    6      0    7          0    7

                  frequency range:        2111        7963
```

```
 Standard errors are obtained by muliplying the previous errors by:   0.562587

 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

        10000         A  /  /MHz        1334.2553(2)                          1
        20000         B  /  /MHz        1209.6121(2)                          2
        30000         C  /  /MHz         893.7174(2)                          3
          200        DJ  /  /kHz         [ 0.048971997]                       4
         2000        DK  /  /kHz         [-0.045366893]                       5
         1100       DJK  /  /kHz         [ 0.046960838]                       6
        40100        d1  /  /kHz         [-0.008933346762]                    7
        50000        d2  /  /kHz         [ 0.003676407495]                    8

 CORRELATION COEFFICIENTS, C.ij:

          A  /     B  /     C  /

A  /        1.0000
B  /        0.7308   1.0000
C  /        0.7080   0.7386   1.0000

 Mean value of |C.ij|, i.ne.j =   0.7258
 Mean value of  C.ij,  i.ne.j =   0.7258


 No correlations with absolute value greater than 0.9950
```

```
 Worst fitted lines (obs-calc/error):

    15:   -1.5        44:   -1.3        24:   -1.3         9:   -1.1
    31:    1.0        49:    0.9        30:    0.9         2:   -0.9
     6:   -0.7        10:    0.7        36:   -0.6        50:    0.6
    38:    0.6        46:   -0.5        22:    0.5         8:    0.5
    21:    0.5        39:    0.4         5:    0.4        27:   -0.4
     1:    0.3        34:   -0.3        41:   -0.3        13:   -0.3
    23:    0.3        33:    0.3        17:    0.2        18:   -0.2
    45:    0.2        48:    0.2         7:    0.1        11:    0.1
    25:   -0.1        28:   -0.1        16:    0.1        35:   -0.1
    20:   -0.1         4:   -0.1        12:   -0.1         3:   -0.1
    47:    0.1        32:   -0.1        19:    0.0        51:    0.0
    29:    0.0        26:    0.0        37:    0.0        42:    0.0
    14:    0.0        43:    0.0

    15:  9  5  4   9  4  5                 2868.2573  -0.0154  0.010
    44:  3  1  2   2  0  2                 7520.8734  -0.0133  0.010
    24:  5  2  4   5  1  5                 3342.3581  -0.0130  0.010
     9:  6  6  1   6  5  2                 2527.4220  -0.0106  0.010
    31:  9  4  6   9  3  7                 4785.5930   0.0096  0.010
    49:  3  2  2   2  1  2                 7631.6040   0.0092  0.010
    30:  2  1  1   1  1  0                 4522.5606   0.0088  0.010
     2:  5  5  1   5  4  2                 2137.9098  -0.0088  0.010
     6:  6  6  0   6  5  1                 2315.2779  -0.0074  0.010
    10:  7  6  2   7  5  3                 2582.0651   0.0073  0.010
-------------------------------------------------------------

C13(9)
```

```
-------------------------------------------------------------------------------=========
                                          obs        o-c     error     blends     Notes
                                                                     o-c      wt
   / instead of : below denotes (o-c)>3*err
-------------------------------------------------------------------------------=========
   1:  5  4  2    5  3  3                 2075.9790   0.0047  0.010
   2:  7  4  3    7  3  4                 2082.9983   0.0065  0.010
   3:  5  5  1    5  4  2                 2117.1239  -0.0036  0.010
   4:  1  1  1    0  0  0                 2223.8461  -0.0072  0.010
   5:  6  5  2    6  4  3                 2279.0569   0.0001  0.010
   6:  6  3  3    6  2  4                 2283.2828   0.0026  0.010
   7:  5  2  3    5  1  4                 2432.6806   0.0098  0.010
   8:  4  2  3    4  1  4                 2547.7367  -0.0147  0.010
   9:  5  3  3    5  2  4                 2551.2210  -0.0014  0.010
  10:  7  6  2    7  5  3                 2553.4864   0.0087  0.010
  11:  6  4  3    6  3  4                 2580.9504   0.0020  0.010
  12:  7  5  3    7  4  4                 2656.0364  -0.0015  0.010
  13:  7  3  4    7  2  5                 3140.4785   0.0029  0.010
  14:  6  2  4    6  1  5                 3221.2890  -0.0088  0.010
  15:  8  5  4    8  4  5                 3225.4411  -0.0136  0.010
  16:  7  4  4    7  3  5                 3230.0056   0.0117  0.010
  17:  6  3  4    6  2  5                 3248.2553   0.0029  0.010
  18:  9  6  4    9  5  5                 3252.4433   0.0035  0.010
  19:  9  8  2    9  7  3                 3283.8546   0.0016  0.010
  20:  2  0  2    1  1  1                 3859.0831   0.0007  0.010
  21:  9  5  5    9  4  6                 3909.3633  -0.0013  0.010
  22:  8  4  5    8  3  6                 3943.9806  -0.0053  0.010
  23:  2  1  2    1  0  1                 4015.1062  -0.0039  0.010
  24:  2  2  1    1  1  0                 4880.2976  -0.0029  0.010
  25:  2  2  0    1  1  1                 5401.4812  -0.0026  0.010
```

```
  26:  3  0  3    2  1  2                        5721.3895  -0.0029  0.010
  27:  3  1  3    2  1  2                        5726.3834  -0.0013  0.010
  28:  3  0  3    2  0  2                        5752.4086  -0.0027  0.010
  29:  3  1  3    2  0  2                        5757.4032  -0.0004  0.010
  30:  3  1  2    2  2  1                        6152.2472   0.0018  0.010
  31:  3  2  2    2  2  1                        6296.5315   0.0042  0.010
  32:  3  1  2    2  1  1                        6527.2724   0.0004  0.010
  33:  4  2  3    3  3  0                        6583.2780   0.0078  0.010
  34:  3  2  2    2  1  1                        6671.5523  -0.0015  0.010
  35:  3  2  1    2  2  0                        6840.6416  -0.0038  0.010
  36:  3  2  1    2  1  1                        7429.2687   0.0000  0.010
  37:  4  0  4    3  1  3                        7527.4315   0.0000  0.010
  38:  4  1  4    3  1  3                        7528.0961   0.0022  0.010
  39:  4  0  4    3  0  3                        7532.4172  -0.0065  0.010
  40:  4  1  4    3  0  3                        7533.0873   0.0010  0.010
  41:  3  3  1    2  2  0                        7585.7058  -0.0009  0.010
  42:  3  3  0    2  2  0                        7707.5810   0.0035  0.010
  43:  3  3  1    2  2  1                        7799.3085   0.0050  0.010
  44:  3  3  0    2  2  1                        7921.1750   0.0008  0.010
--------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated):

        10000         A  /  /MHz        1328.2244(4)                          1
        20000         B  /  /MHz        1203.2156(4)                          2
        30000         C  /  /MHz         895.6290(3)                          3
          200        DJ  /  /kHz         [ 0.048971997]                       4
         2000        DK  /  /kHz         [-0.045366893]                       5
         1100       DJK  /  /kHz         [ 0.046960838]                       6
        40100        d1  /  /kHz         [-0.008933346762]                    7
```

```
       50000        d2  /  /kHz          [ 0.003676407495]                    8

 MICROWAVE AVG =       -0.000054 MHz, IR AVG =       0.00000
 MICROWAVE RMS =        0.005316 MHz, IR RMS =       0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=       0.53161        0.53161

  distinct frequency lines in fit:    44
       distinct parameters of fit:     3

                                    upper state  lower state        overall
      limits of quantum number  1:      1    9      0    9          0    9
      limits of quantum number  2:      0    8      0    7          0    8
      limits of quantum number  3:      0    5      0    6          0    6

                 frequency range:        2075        7921

 Standard errors are obtained by muliplying the previous errors by:   0.550716

 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

       10000         A  /  /MHz         1328.2245(2)                          1
       20000         B  /  /MHz         1203.2157(2)                          2
       30000         C  /  /MHz          895.6290(1)                          3
         200        DJ  /  /kHz          [ 0.048971997]                       4
        2000        DK  /  /kHz          [-0.045366893]                       5
        1100       DJK  /  /kHz          [ 0.046960838]                       6
       40100        d1  /  /kHz          [-0.008933346762]                    7
       50000        d2  /  /kHz          [ 0.003676407495]                    8
```

```
 CORRELATION COEFFICIENTS, C.ij:

           A  /     B  /     C  /

A  /        1.0000
B  /        0.5354   1.0000
C  /        0.6229   0.6263   1.0000

 Mean value of |C.ij|, i.ne.j =   0.5948
 Mean value of  C.ij,  i.ne.j =   0.5948


 No correlations with absolute value greater than 0.9950


 Worst fitted lines (obs-calc/error):

    8:   -1.5        15:   -1.4        16:    1.2         7:    1.0
   14:   -0.9        10:    0.9        33:    0.8         4:   -0.7
    2:    0.6        39:   -0.6        22:   -0.5        43:    0.5
    1:    0.5        31:    0.4        23:   -0.4        35:   -0.4
    3:   -0.4        18:    0.3        42:    0.3        26:   -0.3
   17:    0.3        24:   -0.3        13:    0.3        28:   -0.3
    6:    0.3        25:   -0.3        38:    0.2        11:    0.2
   30:    0.2        19:    0.2        12:   -0.1        34:   -0.1
    9:   -0.1        21:   -0.1        27:   -0.1        40:    0.1
   41:   -0.1        44:    0.1        20:    0.1        32:    0.0
   29:    0.0         5:    0.0        37:    0.0        36:    0.0

    8:  4  2  3    4  1  4                   2547.7367  -0.0147  0.010
```

```
    15:  8  5  4    8  4  5                     3225.4411  -0.0136  0.010
    16:  7  4  4    7  3  5                     3230.0056   0.0117  0.010
     7:  5  2  3    5  1  4                     2432.6806   0.0098  0.010
    14:  6  2  4    6  1  5                     3221.2890  -0.0088  0.010
    10:  7  6  2    7  5  3                     2553.4864   0.0087  0.010
    33:  4  2  3    3  3  0                     6583.2780   0.0078  0.010
     4:  1  1  1    0  0  0                     2223.8461  -0.0072  0.010
     2:  7  4  3    7  3  4                     2082.9983   0.0065  0.010
    39:  4  0  4    3  0  3                     7532.4172  -0.0065  0.010
------------------------------------------------------------


C13(12)

--------------------------------------------------------------------------------------=========
                                               obs         o-c     error     blends     Notes
                                                                               o-c      wt
    / instead of : below denotes (o-c)>3*err
--------------------------------------------------------------------------------------=========
   1:  5  4  2    5  3  3                     2120.5252   0.0012  0.010
   2:  7  4  3    7  3  4                     2145.4766  -0.0075  0.010
   3:  5  5  1    5  4  2                     2153.3784  -0.0053  0.010
   4:  1  1  1    0  0  0                     2206.5470   0.0000  0.010
   5:  6  5  2    6  4  3                     2323.8580   0.0054  0.010
   6:  6  6  0    6  5  1                     2338.9918  -0.0113  0.010
   7:  6  3  3    6  2  4                     2347.7616  -0.0020  0.010
   8:  5  2  3    5  1  4                     2496.8183  -0.0028  0.010
   9:  6  6  1    6  5  2                     2547.3969  -0.0105  0.010
  10:  4  1  3    4  0  4                     2578.2427   0.0178  0.010
  11:  7  6  2    7  5  3                     2599.2341  -0.0024  0.010
```

12:	4	2	3	4	1	4	2610.6105	-0.0108	0.010
13:	5	3	3	5	2	4	2613.6452	0.0061	0.010
14:	6	4	3	6	3	4	2642.4458	-0.0002	0.010
15:	7	5	3	7	4	4	2716.1795	0.0071	0.010
16:	8	6	3	8	5	4	2851.6629	0.0092	0.010
17:	9	5	4	9	4	5	2862.4114	-0.0146	0.010
18:	8	7	2	8	6	3	2940.5118	0.0037	0.010
19:	9	8	1	9	7	2	3068.6487	0.0042	0.010
20:	8	4	4	8	3	5	3079.9493	-0.0095	0.010
21:	7	3	4	7	2	5	3223.3731	0.0032	0.010
22:	6	2	4	6	1	5	3303.0478	-0.0003	0.010
23:	7	4	4	7	3	5	3310.3996	0.0021	0.010
24:	6	3	4	6	2	5	3329.1775	0.0013	0.010
25:	9	6	4	9	5	5	3329.6274	0.0043	0.010
26:	9	8	2	9	7	3	3335.0425	0.0029	0.010
27:	5	1	4	5	0	5	3343.1372	0.0067	0.010
28:	5	2	4	5	1	5	3348.6890	0.0066	0.010
29:	2	0	2	1	1	1	3813.8099	-0.0063	0.010
30:	9	4	5	9	3	6	3947.5452	0.0019	0.010
31:	2	1	2	1	0	1	3970.9146	-0.0016	0.010
32:	9	5	5	9	4	6	4008.0510	-0.0020	0.010
33:	8	4	5	8	3	6	4043.1008	0.0022	0.010
34:	7	3	5	7	2	6	4073.4151	0.0080	0.010
35:	2	2	1	1	1	0	4855.2693	0.0002	0.010
36:	2	1	1	1	0	1	4918.7941	-0.0145	0.010
37:	2	2	1	1	1	1	5171.2274	-0.0059	0.010
38:	2	2	0	1	1	1	5391.8729	-0.0002	0.010
39:	7	6	1	7	3	4	5518.4147	-0.0112	0.010
40:	3	0	3	2	1	2	5649.8536	-0.0035	0.010
41:	3	0	3	2	0	2	5680.7369	-0.0079	0.010

```
  42:  3  1  3    2  0  2                         5685.6426  -0.0002  0.010
  43:  3  1  2    2  2  1                         6097.0852   0.0106  0.010
  44:  3  1  2    2  1  1                         6475.7054  -0.0061  0.010
  45:  3  2  2    2  1  1                         6619.6369   0.0020  0.010
  46:  3  2  1    2  2  0                         6801.2552   0.0020  0.010
  47:  3  2  1    2  1  1                         7400.5284  -0.0014  0.010
  48:  4  0  4    3  1  3                         7428.9421  -0.0007  0.010
  49:  4  0  4    3  0  3                         7433.8538   0.0129  0.010
  50:  4  1  4    3  0  3                         7434.4837   0.0023  0.010
  51:  3  3  1    2  2  0                         7553.6309   0.0015  0.010
  52:  3  3  0    2  2  0                         7680.5610  -0.0031  0.010
  53:  3  3  1    2  2  1                         7774.2737   0.0044  0.010
  54:  3  3  0    2  2  1                         7901.2054   0.0014  0.010
--------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated):

        10000         A  /  /MHz         1324.3619(4)                         1
        20000         B  /  /MHz         1198.1496(4)                         2
        30000         C  /  /MHz          882.1852(3)                         3
          200        DJ  /  /kHz          [ 0.048971997]                      4
         2000        DK  /  /kHz          [-0.045366893]                      5
         1100       DJK  /  /kHz          [ 0.046960838]                      6
        40100        d1  /  /kHz          [-0.008933346762]                   7
        50000        d2  /  /kHz          [ 0.003676407495]                   8

 MICROWAVE AVG =       -0.000197 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.006660 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=       0.66597         0.66597
```

```
 distinct frequency lines in fit:    54
      distinct parameters of fit:     3

                                    upper state  lower state         overall
     limits of quantum number  1:      1    9       0    9           0    9
     limits of quantum number  2:      0    8       0    7           0    8
     limits of quantum number  3:      0    5       0    6           0    6

                 frequency range:        2120         7901

Standard errors are obtained by muliplying the previous errors by:   0.685277

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

       10000         A  /  /MHz        1324.3619(2)                        1
       20000         B  /  /MHz        1198.1496(2)                        2
       30000         C  /  /MHz         882.1853(2)                        3
         200        DJ  /  /kHz         [ 0.048971997]                     4
        2000        DK  /  /kHz         [-0.045366893]                     5
        1100       DJK  /  /kHz         [ 0.046960838]                     6
       40100        d1  /  /kHz         [-0.008933346762]                  7
       50000        d2  /  /kHz         [ 0.003676407495]                  8

CORRELATION COEFFICIENTS, C.ij:

          A  /     B  /     C  /

A  /        1.0000
B  /        0.8322   1.0000
```

```
C  /        0.8024   0.8087   1.0000

 Mean value of |C.ij|, i.ne.j =   0.8144
 Mean value of  C.ij,  i.ne.j =   0.8144


 No correlations with absolute value greater than 0.9950


 Worst fitted lines (obs-calc/error):

    10:    1.8         17:   -1.5         36:   -1.4         49:    1.3
     6:   -1.1         39:   -1.1         12:   -1.1         43:    1.1
     9:   -1.1         20:   -0.9         16:    0.9         34:    0.8
    41:   -0.8          2:   -0.8         15:    0.7         27:    0.7
    28:    0.7         29:   -0.6         13:    0.6         44:   -0.6
    37:   -0.6          5:    0.5          3:   -0.5         53:    0.4
    25:    0.4         19:    0.4         18:    0.4         40:   -0.3
    21:    0.3         52:   -0.3         26:    0.3          8:   -0.3
    11:   -0.2         50:    0.2         33:    0.2         23:    0.2
    46:    0.2         45:    0.2          7:   -0.2         32:   -0.2
    30:    0.2         31:   -0.2         51:    0.1         54:    0.1
    47:   -0.1         24:    0.1          1:    0.1         48:   -0.1
    22:    0.0         42:    0.0

    10:  4  1  3   4  0  4                   2578.2427   0.0178  0.010
    17:  9  5  4   9  4  5                   2862.4114  -0.0146  0.010
    36:  2  1  1   1  0  1                   4918.7941  -0.0145  0.010
    49:  4  0  4   3  0  3                   7433.8538   0.0129  0.010
     6:  6  6  0   6  5  1                   2338.9918  -0.0113  0.010
```

```
   39:  7  6  1    7  3  4                    5518.4147  -0.0112  0.010
   12:  4  2  3    4  1  4                    2610.6105  -0.0108  0.010
   43:  3  1  2    2  2  1                    6097.0852   0.0106  0.010
    9:  6  6  1    6  5  2                    2547.3969  -0.0105  0.010
   20:  8  4  4    8  3  5                    3079.9493  -0.0095  0.010
---------------------------------------------------------

C13(16)

-----------------------------------------------------------------------------------------=========
                                              obs         o-c     error     blends     Notes
                                                                          o-c      wt
    / instead of : below denotes (o-c)>3*err
-----------------------------------------------------------------------------------------=========
  1:  4  3  2    4  2  3                    2020.0180   0.0014  0.010
  2:  5  5  0    5  4  1                    2021.5848  -0.0006  0.010
  3:  7  4  3    7  3  4                    2034.3847   0.0037  0.010
  4:  5  4  2    5  3  3                    2189.7597   0.0019  0.010
  5:  1  1  1    0  0  0                    2221.3917   0.0024  0.010
  6:  7  6  1    7  5  2                    2223.5543   0.0020  0.010
  7:  6  3  3    6  2  4                    2258.9194  -0.0052  0.010
  8:  5  5  1    5  4  2                    2315.7290  -0.0024  0.010
  9:  5  2  3    5  1  4                    2448.1578   0.0017  0.010
 10:  4  1  3    4  0  4                    2559.2951   0.0130  0.010
 11:  4  2  3    4  1  4                    2607.6941  -0.0129  0.010
 12:  5  3  3    5  2  4                    2617.3740  -0.0004  0.010
 13:  6  4  3    6  3  4                    2665.2503  -0.0013  0.010
 14:  6  6  1    6  5  2                    2762.6967   0.0078  0.010
 15:  7  5  3    7  4  4                    2774.7809   0.0013  0.010
 16:  7  6  2    7  5  3                    2777.9860   0.0035  0.010
```

17:	8	7	1	8	6	2	2848.2378	-0.0034	0.010
18:	8	6	3	8	5	4	2963.5580	-0.0017	0.010
19:	7	3	4	7	2	5	3157.5818	0.0013	0.010
20:	8	7	2	8	6	3	3182.7569	0.0054	0.010
21:	9	7	3	9	6	4	3238.5948	-0.0029	0.010
22:	7	7	1	7	6	2	3244.3261	0.0013	0.010
23:	6	2	4	6	1	5	3272.9226	0.0137	0.010
24:	7	4	4	7	3	5	3300.8212	0.0023	0.010
25:	8	5	4	8	4	5	3309.2681	-0.0014	0.010
26:	6	3	4	6	2	5	3317.3480	0.0017	0.010
27:	5	2	4	5	1	5	3339.9387	0.0029	0.010
28:	9	8	2	9	7	3	3639.0030	0.0022	0.010
29:	2	0	2	1	1	1	3803.6683	-0.0020	0.010
30:	9	4	5	9	3	6	3868.1250	-0.0013	0.010
31:	2	0	2	1	0	1	3949.1329	0.0026	0.010
32:	9	5	5	9	4	6	3981.6326	0.0041	0.010
33:	8	3	5	8	2	6	3982.7733	-0.0086	0.010
34:	2	1	2	1	0	1	3989.7750	0.0004	0.010
35:	8	4	5	8	3	6	4019.4056	-0.0037	0.010
36:	7	2	5	7	1	6	4047.1265	0.0051	0.010
37:	7	3	5	7	2	6	4056.2924	-0.0039	0.010
38:	2	1	1	1	1	0	4459.4020	0.0020	0.010
39:	2	2	1	1	1	0	4895.7788	-0.0011	0.010
40:	6	5	1	6	2	4	5316.3355	-0.0082	0.010
41:	2	2	0	1	1	1	5406.0495	-0.0007	0.010
42:	3	0	3	2	1	2	5655.3236	-0.0033	0.010
43:	3	1	3	2	1	2	5662.7624	-0.0039	0.010
44:	3	0	3	2	0	2	5695.9657	-0.0054	0.010
45:	3	1	3	2	0	2	5703.4095	-0.0011	0.010
46:	3	1	2	2	2	1	6041.8620	0.0055	0.010

```
 47:  3  2  2    2  2  1                          6227.7814  -0.0005  0.010
 48:  4  2  3    3  3  0                          6420.9239   0.0161  0.010
 49:  3  1  2    2  1  1                          6478.2360  -0.0002  0.010
 50:  3  2  2    2  1  1                          6664.1615  -0.0003  0.010
 51:  3  2  1    2  2  0                          6759.5954   0.0007  0.010
 52:  3  2  1    2  1  1                          7398.7049   0.0029  0.010
 53:  4  0  4    3  1  3                          7443.1158  -0.0052  0.010
 54:  4  1  4    3  1  3                          7444.2432   0.0008  0.010
 55:  4  0  4    3  0  3                          7450.5570  -0.0035  0.010
 56:  4  1  4    3  0  3                          7451.6848   0.0029  0.010
 57:  3  2  2    2  1  2                          7586.7792  -0.0108  0.010
 58:  3  3  1    2  2  0                          7624.9150  -0.0003  0.010
 59:  3  3  0    2  2  1                          7934.8004   0.0005  0.010
--------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated):

       10000         A  /  /MHz         1337.1962(3)                         1
       20000         B  /  /MHz         1191.7362(3)                         2
       30000         C  /  /MHz          884.1932(3)                         3
         200        DJ  /  /kHz          [ 0.048971997]                      4
        2000        DK  /  /kHz          [-0.045366893]                      5
        1100       DJK  /  /kHz          [ 0.046960838]                      6
       40100        d1  /  /kHz          [-0.008933346762]                   7
       50000        d2  /  /kHz          [ 0.003676407495]                   8

 MICROWAVE AVG =        0.000286 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.005064 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=       0.50640         0.50640
```

```
 distinct frequency lines in fit:    59
      distinct parameters of fit:     3

                                  upper state  lower state         overall
     limits of quantum number  1:      1    9       0    9           0    9
     limits of quantum number  2:      0    8       0    7           0    8
     limits of quantum number  3:      0    5       0    6           0    6

                frequency range:        2020        7934

Standard errors are obtained by muliplying the previous errors by:   0.519787

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

        10000         A  /  /MHz        1337.1962(1)                        1
        20000         B  /  /MHz        1191.7363(1)                        2
        30000         C  /  /MHz         884.1933(1)                        3
          200        DJ  /  /kHz         [ 0.048971997]                     4
         2000        DK  /  /kHz         [-0.045366893]                     5
         1100       DJK  /  /kHz         [ 0.046960838]                     6
        40100        d1  /  /kHz         [-0.008933346762]                  7
        50000        d2  /  /kHz         [ 0.003676407495]                  8

CORRELATION COEFFICIENTS, C.ij:

           A  /     B  /     C  /

A  /        1.0000
B  /        0.8180   1.0000
```

```
C  /        0.7841   0.7692   1.0000

 Mean value of |C.ij|, i.ne.j =   0.7904
 Mean value of  C.ij,  i.ne.j =   0.7904


 No correlations with absolute value greater than 0.9950


 Worst fitted lines (obs-calc/error):

    48:    1.6         23:    1.4         10:    1.3         11:   -1.3
    57:   -1.1         33:   -0.9         40:   -0.8         14:    0.8
    46:    0.5         44:   -0.5         20:    0.5          7:   -0.5
    53:   -0.5         36:    0.5         32:    0.4         37:   -0.4
    43:   -0.4          3:    0.4         35:   -0.4         16:    0.3
    55:   -0.3         17:   -0.3         42:   -0.3         52:    0.3
    21:   -0.3         56:    0.3         27:    0.3         31:    0.3
     5:    0.2          8:   -0.2         24:    0.2         28:    0.2
     6:    0.2         38:    0.2         29:   -0.2          4:    0.2
    26:    0.2          9:    0.2         18:   -0.2         25:   -0.1
     1:    0.1         13:   -0.1         30:   -0.1         22:    0.1
    19:    0.1         15:    0.1         39:   -0.1         45:   -0.1
    54:    0.1         51:    0.1

    48:  4  2  3   3  3  0                    6420.9239   0.0161  0.010
    23:  6  2  4   6  1  5                    3272.9226   0.0137  0.010
    10:  4  1  3   4  0  4                    2559.2951   0.0130  0.010
    11:  4  2  3   4  1  4                    2607.6941  -0.0129  0.010
    57:  3  2  2   2  1  2                    7586.7792  -0.0108  0.010
```

```
    33:  8  3  5    8  2  6                         3982.7733  -0.0086  0.010
    40:  6  5  1    6  2  4                         5316.3355  -0.0082  0.010
    14:  6  6  1    6  5  2                         2762.6967   0.0078  0.010
    46:  3  1  2    2  2  1                         6041.8620   0.0055  0.010
    44:  3  0  3    2  0  2                         5695.9657  -0.0054  0.010
----------------------------------------------------------

C13(20)

---------------------------------------------------------------------------------------=========
                                              obs          o-c      error     blends     Notes
                                                                              o-c      wt
    / instead of : below denotes (o-c)>3*err
---------------------------------------------------------------------------------------=========
   1:  3  3  0    2  2  1                         7907.2272   0.0002  0.010
   2:  3  3  1    2  2  1                         7788.7826   0.0014  0.010
   3:  3  3  0    2  2  0                         7696.9448   0.0029  0.010
   4:  3  2  2    2  1  2                         7579.3948   0.0148  0.010
   5:  3  3  1    2  2  0                         7578.4957  -0.0004  0.010
   6:  4  1  4    3  0  3                         7519.3552   0.0012  0.010
   7:  4  0  4    3  0  3                         7518.6304  -0.0016  0.010
   8:  4  1  4    3  1  3                         7514.0343  -0.0003  0.010
   9:  4  0  4    3  1  3                         7513.3112  -0.0014  0.010
  10:  3  2  1    2  1  1                         7411.6347  -0.0050  0.010
  11:  3  2  1    2  2  0                         6818.8965   0.0022  0.010
  12:  3  2  2    2  1  1                         6662.9910  -0.0008  0.010
  13:  4  2  3    3  3  0                         6563.1903   0.0032  0.010
  14:  3  1  2    2  1  1                         6513.1205  -0.0016  0.010
  15:  3  2  2    2  2  1                         6280.5149  -0.0165  0.010
  16:  3  1  2    2  2  1                         6130.6762   0.0144  0.010
```

17:	3	1	3	2	0	2	5747.4896	-0.0004	0.010
18:	3	0	3	2	0	2	5742.1635	-0.0072	0.010
19:	3	1	3	2	1	2	5715.1799	-0.0012	0.010
20:	3	0	3	2	1	2	5709.8669	0.0050	0.010
21:	2	2	0	1	1	1	5390.6917	-0.0030	0.010
22:	2	2	0	1	1	0	5085.2258	-0.0060	0.010
23:	2	2	1	1	1	0	4874.9454	-0.0013	0.010
24:	2	1	1	1	1	0	4492.4803	-0.0060	0.010
25:	2	1	2	1	0	1	4009.0442	-0.0036	0.010
26:	2	0	2	1	0	1	3976.7478	0.0088	0.010
27:	2	0	2	1	1	1	3849.2522	0.0000	0.010
28:	1	1	1	0	0	0	2220.9939	-0.0054	0.010
29:	8	5	4	8	4	5	3216.4490	0.0042	0.010
30:	7	4	4	7	3	5	3219.2164	0.0020	0.010
31:	6	3	4	6	2	5	3237.2516	-0.0020	0.010
32:	9	6	4	9	5	5	3247.6336	0.0040	0.010
33:	9	4	5	9	3	6	3824.5886	-0.0098	0.010
34:	9	5	5	9	4	6	3894.2029	0.0018	0.010
35:	8	4	5	8	3	6	3929.3178	0.0074	0.010
36:	7	3	5	7	2	6	3960.4743	0.0014	0.010
37:	9	8	2	9	7	3	3319.2524	-0.0014	0.010
38:	6	2	4	6	1	5	3208.0014	-0.0005	0.010
39:	7	3	4	7	2	5	3122.5251	0.0059	0.010
40:	9	8	1	9	7	2	3085.3440	0.0081	0.010
41:	8	7	2	8	6	3	2919.8520	-0.0071	0.010
42:	7	7	0	7	6	1	2869.0504	-0.0029	0.010
43:	7	5	3	7	4	4	2656.4534	-0.0047	0.010
44:	6	4	3	6	3	4	2576.5987	0.0004	0.010
45:	5	3	3	5	2	4	2544.3662	-0.0029	0.010
46:	4	2	3	4	1	4	2540.0343	-0.0124	0.010

```
 47:  5  2  3    5  1  4                    2418.9183   0.0017  0.010
 48:  6  3  3    6  2  4                    2263.8997  -0.0008  0.010
 49:  5  5  1    5  4  2                    2134.9988   0.0021  0.010
 50:  5  4  2    5  3  3                    2079.9521   0.0013  0.010
--------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated):

      10000         A  /  /MHz        1326.9746(3)                          1
      20000         B  /  /MHz        1199.4878(3)                          2
      30000         C  /  /MHz         894.0249(3)                          3
        200        DJ  /  /kHz         [ 0.048971997]                       4
       2000        DK  /  /kHz         [-0.045366893]                       5
       1100       DJK  /  /kHz         [ 0.046960838]                       6
      40100        d1  /  /kHz         [-0.008933346762]                    7
      50000        d2  /  /kHz         [ 0.003676407495]                    8

 MICROWAVE AVG =       -0.000240 MHz, IR AVG =       0.00000
 MICROWAVE RMS =        0.005672 MHz, IR RMS =       0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=       0.56721         0.56721

  distinct frequency lines in fit:    50
       distinct parameters of fit:     3

                                    upper state  lower state        overall
      limits of quantum number  1:      1    9       0    9          0    9
      limits of quantum number  2:      0    8       0    7          0    8
      limits of quantum number  3:      0    5       0    6          0    6

                  frequency range:        2079        7907
```

```
 Standard errors are obtained by muliplying the previous errors by:   0.585032

 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

        10000         A  /  /MHz        1326.9746(2)                         1
        20000         B  /  /MHz        1199.4878(2)                         2
        30000         C  /  /MHz         894.0249(1)                         3
          200        DJ  /  /kHz         [ 0.048971997]                      4
         2000        DK  /  /kHz         [-0.045366893]                      5
         1100       DJK  /  /kHz         [ 0.046960838]                      6
        40100        d1  /  /kHz         [-0.008933346762]                   7
        50000        d2  /  /kHz         [ 0.003676407495]                   8

 CORRELATION COEFFICIENTS, C.ij:

           A  /     B  /     C  /

A  /        1.0000
B  /        0.7303   1.0000
C  /        0.6777   0.6727   1.0000

 Mean value of |C.ij|, i.ne.j =   0.6936
 Mean value of  C.ij,  i.ne.j =   0.6936


 No correlations with absolute value greater than 0.9950
```

```
 Worst fitted lines (obs-calc/error):

    15:   -1.7          4:    1.5         16:    1.4         46:   -1.2
    33:   -1.0         26:    0.9         40:    0.8         35:    0.7
    18:   -0.7         41:   -0.7         24:   -0.6         22:   -0.6
    39:    0.6         28:   -0.5         20:    0.5         10:   -0.5
    43:   -0.5         29:    0.4         32:    0.4         25:   -0.4
    13:    0.3         21:   -0.3         42:   -0.3         45:   -0.3
     3:    0.3         11:    0.2         49:    0.2         31:   -0.2
    30:    0.2         34:    0.2         47:    0.2         14:   -0.2
     7:   -0.2         37:   -0.1         36:    0.1          2:    0.1
     9:   -0.1         50:    0.1         23:   -0.1         19:   -0.1
     6:    0.1         48:   -0.1         12:   -0.1         38:   -0.1
    44:    0.0          5:    0.0         17:    0.0          8:    0.0
     1:    0.0         27:    0.0

    15:  3  2  2   2  2  1                    6280.5149  -0.0165  0.010
     4:  3  2  2   2  1  2                    7579.3948   0.0148  0.010
    16:  3  1  2   2  2  1                    6130.6762   0.0144  0.010
    46:  4  2  3   4  1  4                    2540.0343  -0.0124  0.010
    33:  9  4  5   9  3  6                    3824.5886  -0.0098  0.010
    26:  2  0  2   1  0  1                    3976.7478   0.0088  0.010
    40:  9  8  1   9  7  2                    3085.3440   0.0081  0.010
    35:  8  4  5   8  3  6                    3929.3178   0.0074  0.010
    18:  3  0  3   2  0  2                    5742.1635  -0.0072  0.010
    41:  8  7  2   8  6  3                    2919.8520  -0.0071  0.010
-------------------------------------------------------------

C13(24)
```

```
-----------------------------------------------------------------------------------=========
                                             obs         o-c     error     blends     Notes
                                                                          o-c      wt
    / instead of : below denotes (o-c)>3*err
-----------------------------------------------------------------------------------=========
   1:  5  4  2    5  3  3                    2102.5342   0.0003  0.010
   2:  5  5  1    5  4  2                    2105.9447   0.0018  0.010
   3:  7  4  3    7  3  4                    2183.1844  -0.0026  0.010
   4:  1  1  1    0  0  0                    2223.3967   0.0000  0.010
   5:  6  5  2    6  4  3                    2291.3623   0.0024  0.010
   6:  6  3  3    6  2  4                    2375.5240  -0.0029  0.010
   7:  8  7  1    8  6  2                    2378.4405   0.0062  0.010
   8:  6  6  1    6  5  2                    2483.6983  -0.0052  0.010
   9:  4  1  3    4  0  4                    2585.3893   0.0178  0.010
  10:  5  3  3    5  2  4                    2615.1885   0.0181  0.010
  11:  6  4  3    6  3  4                    2639.1254  -0.0011  0.010
  12:  7  5  3    7  4  4                    2703.2626  -0.0117  0.010
  13:  8  6  3    8  5  4                    2823.8949   0.0021  0.010
  14:  8  7  2    8  6  3                    2870.7145  -0.0042  0.010
  15:  8  4  4    8  3  5                    3115.4925   0.0007  0.010
  16:  7  3  4    7  2  5                    3243.1675   0.0017  0.010
  17:  9  8  2    9  7  3                    3245.7652   0.0004  0.010
  18:  8  5  4    8  4  5                    3307.9237   0.0000  0.010
  19:  7  4  4    7  3  5                    3316.6195  -0.0009  0.010
  20:  9  6  4    9  5  5                    3325.0791  -0.0072  0.010
  21:  6  3  4    6  2  5                    3335.4561   0.0010  0.010
  22:  5  1  4    5  0  5                    3349.2531   0.0001  0.010
  23:  5  2  4    5  1  5                    3353.8770   0.0023  0.010
  24:  2  0  2    1  1  1                    3858.8312  -0.0022  0.010
  25:  9  4  5    9  3  6                    3970.9143   0.0038  0.010
```

```
 26:  2  1  2    1  0  1                         4007.5104   0.0021  0.010
 27:  9  5  5    9  4  6                         4019.7529  -0.0095  0.010
 28:  8  4  5    8  3  6                         4053.3184  -0.0020  0.010
 29:  7  2  5    7  1  6                         4077.8300   0.0039  0.010
 30:  2  1  1    1  1  0                         4524.6320  -0.0077  0.010
 31:  2  2  1    1  1  0                         4886.0752  -0.0009  0.010
 32:  2  2  0    1  1  0                         5112.5906  -0.0082  0.010
 33:  6  5  1    6  2  4                         5193.3858  -0.0043  0.010
 34:  2  2  0    1  1  1                         5431.4034  -0.0007  0.010
 35:  3  0  3    2  1  2                         5711.1516  -0.0011  0.010
 36:  3  1  3    2  1  2                         5715.4175   0.0021  0.010
 37:  3  0  3    2  0  2                         5739.3410  -0.0077  0.010
 38:  3  1  3    2  0  2                         5743.6122   0.0007  0.010
 39:  3  1  2    2  2  1                         6176.6615   0.0072  0.010
 40:  3  2  2    2  2  1                         6308.7499   0.0021  0.010
 41:  3  1  2    2  1  1                         6538.0900  -0.0006  0.010
 42:  3  2  2    2  1  1                         6670.1841  -0.0001  0.010
 43:  3  2  1    2  2  0                         6878.1479  -0.0010  0.010
 44:  3  2  1    2  1  1                         7466.1071  -0.0009  0.010
 45:  4  0  4    3  1  3                         7508.6940   0.0050  0.010
 46:  4  0  4    3  0  3                         7512.9519   0.0002  0.010
 47:  4  1  4    3  0  3                         7513.4831  -0.0001  0.010
 48:  3  3  1    2  2  0                         7596.7607   0.0011  0.010
 49:  3  3  0    2  2  0                         7730.5010   0.0025  0.010
 50:  3  3  0    2  2  1                         7957.0218   0.0006  0.010
--------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated):

        10000         A  /  /MHz         1331.3405(4)                          1
```

```
         20000          B  /  /MHz         1210.8617(4)                        2
         30000          C  /  /MHz          892.0564(3)                        3
           200         DJ  /  /kHz          [ 0.048971997]                     4
          2000         DK  /  /kHz          [-0.045366893]                     5
          1100        DJK  /  /kHz          [ 0.046960838]                     6
         40100         d1  /  /kHz          [-0.008933346762]                  7
         50000         d2  /  /kHz          [ 0.003676407495]                  8

 MICROWAVE AVG =        0.000075 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.005306 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.53063         0.53063

  distinct frequency lines in fit:    50
       distinct parameters of fit:     3

                                   upper state  lower state        overall
      limits of quantum number  1:      1    9       0    9          0    9
      limits of quantum number  2:      0    8       0    7          0    8
      limits of quantum number  3:      0    5       0    6          0    6

                 frequency range:        2102         7957

 Standard errors are obtained by muliplying the previous errors by:   0.547303

 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

         10000          A  /  /MHz         1331.3406(2)                        1
         20000          B  /  /MHz         1210.8618(2)                        2
         30000          C  /  /MHz          892.0564(2)                        3
```

```
         200        DJ  /  /kHz          [ 0.048971997]                     4
        2000        DK  /  /kHz          [-0.045366893]                     5
        1100       DJK  /  /kHz          [ 0.046960838]                     6
       40100        d1  /  /kHz          [-0.008933346762]                  7
       50000        d2  /  /kHz          [ 0.003676407495]                  8

 CORRELATION COEFFICIENTS, C.ij:

          A  /     B  /     C  /

A  /        1.0000
B  /        0.7544   1.0000
C  /        0.7611   0.7703   1.0000

 Mean value of |C.ij|, i.ne.j =   0.7619
 Mean value of  C.ij,  i.ne.j =   0.7619


 No correlations with absolute value greater than 0.9950


 Worst fitted lines (obs-calc/error):

    10:    1.8          9:    1.8         12:   -1.2         27:   -0.9
    32:   -0.8         30:   -0.8         37:   -0.8         20:   -0.7
    39:    0.7          7:    0.6          8:   -0.5         45:    0.5
    33:   -0.4         14:   -0.4         29:    0.4         25:    0.4
     6:   -0.3          3:   -0.3         49:    0.2          5:    0.2
    23:    0.2         24:   -0.2         40:    0.2         13:    0.2
    36:    0.2         26:    0.2         28:   -0.2          2:    0.2
```

```
    16:    0.2          35:   -0.1          48:    0.1          11:   -0.1
    43:   -0.1          21:    0.1          44:   -0.1          31:   -0.1
    19:   -0.1          34:   -0.1          15:    0.1          38:    0.1
    50:    0.1          41:   -0.1          17:    0.0           1:    0.0
    46:    0.0          47:    0.0          42:    0.0          22:    0.0
    18:    0.0           4:    0.0

    10:  5  3  3   5  2  4                    2615.1885   0.0181  0.010
     9:  4  1  3   4  0  4                    2585.3893   0.0178  0.010
    12:  7  5  3   7  4  4                    2703.2626  -0.0117  0.010
    27:  9  5  5   9  4  6                    4019.7529  -0.0095  0.010
    32:  2  2  0   1  1  0                    5112.5906  -0.0082  0.010
    30:  2  1  1   1  1  0                    4524.6320  -0.0077  0.010
    37:  3  0  3   2  0  2                    5739.3410  -0.0077  0.010
    20:  9  6  4   9  5  5                    3325.0791  -0.0072  0.010
    39:  3  1  2   2  2  1                    6176.6615   0.0072  0.010
     7:  8  7  1   8  6  2                    2378.4405   0.0062  0.010
-------------------------------------------------------------------

 O18(25)

-------------------------------------------------------------------------------------=========
                                              obs         o-c     error     blends     Notes
                                                                             o-c      wt
    / instead of : below denotes (o-c)>3*err
-------------------------------------------------------------------------------------=========
   1:  5  2  3   5  1  4                    2569.4580  -0.0107  0.010
   2:  8  5  4   8  4  5                    3320.8224  -0.0037  0.010
   3:  7  4  4   7  3  5                    3336.0583   0.0002  0.010
   4:  2  0  2   1  1  1                    3809.1086  -0.0004  0.010
```

```
    5:  2  1  2    1  1  1                     3824.5886   0.0206  0.010
    6:  2  1  2    1  0  1                     3913.2046   0.0135  0.010
    7:  7  3  5    7  1  6                     4100.8327   0.0138  0.010
    8:  2  2  1    1  1  0                     4756.1703   0.0018  0.010
    9:  2  2  0    1  1  1                     5348.7281  -0.0078  0.010
   10:  3  0  3    2  1  2                     5604.0652  -0.0006  0.010
   11:  3  1  3    2  1  2                     5605.7733  -0.0091  0.010
   12:  3  0  3    2  0  2                     5619.5165  -0.0082  0.010
   13:  3  1  3    2  0  2                     5621.2452   0.0039  0.010
   14:  9  8  1    9  5  4                     5779.8948  -0.0002  0.010
   15:  3  1  2    2  2  1                     6161.7329   0.0028  0.010
   16:  3  2  2    2  2  1                     6236.1417  -0.0043  0.010
   17:  3  1  2    2  1  1                     6427.5960  -0.0035  0.010
   18:  3  2  2    2  1  1                     6502.0159   0.0003  0.010
   19:  3  2  1    2  2  0                     6852.7711   0.0014  0.010
   20:  4  0  4    3  1  3                     7357.2490  -0.0001  0.010
   21:  4  1  4    3  1  3                     7357.4090   0.0022  0.010
   22:  4  0  4    3  0  3                     7358.9593  -0.0063  0.010
   23:  4  1  4    3  0  3                     7359.1292   0.0059  0.010
   24:  3  3  1    2  2  0                     7382.7923   0.0000  0.010
   25:  3  3  0    2  2  1                     7819.2689  -0.0035  0.010
-------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated):

        10000         A  /  /MHz         1294.4148(4)                      1
        20000         B  /  /MHz         1205.7917(5)                      2
        30000         C  /  /MHz          872.9258(4)                      3
          200        DJ  /  /kHz          [ 0.048971997]                   4
         2000        DK  /  /kHz          [-0.045366893]                   5
```

```
        1100       DJK  /  /kHz          [ 0.046960838]                    6
       40100        d1  /  /kHz          [-0.008933346762]                 7
       50000        d2  /  /kHz          [ 0.003676407495]                 8

MICROWAVE AVG =        0.000326 MHz, IR AVG =        0.00000
MICROWAVE RMS =        0.007209 MHz, IR RMS =        0.00000
END OF ITERATION  1 OLD, NEW RMS ERROR=        0.72085         0.72085

 distinct frequency lines in fit:    25
      distinct parameters of fit:     3

                                   upper state  lower state        overall
     limits of quantum number  1:      2    9       1    9           1    9
     limits of quantum number  2:      0    8       0    5           0    8
     limits of quantum number  3:      0    5       0    6           0    6

                 frequency range:        2569        7819

Standard errors are obtained by muliplying the previous errors by:   0.768429

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

       10000         A  /  /MHz         1294.4149(3)                       1
       20000         B  /  /MHz         1205.7917(4)                       2
       30000         C  /  /MHz          872.9259(3)                       3
         200        DJ  /  /kHz          [ 0.048971997]                    4
        2000        DK  /  /kHz          [-0.045366893]                    5
        1100       DJK  /  /kHz          [ 0.046960838]                    6
       40100        d1  /  /kHz          [-0.008933346762]                 7
```

```
       50000        d2  /  /kHz          [ 0.003676407495]                    8

 CORRELATION COEFFICIENTS, C.ij:

           A  /     B  /     C  /

A  /        1.0000
B  /        0.6693   1.0000
C  /        0.5055   0.3092   1.0000

 Mean value of |C.ij|, i.ne.j =   0.4946
 Mean value of  C.ij,  i.ne.j =   0.4946


 No correlations with absolute value greater than 0.9950


 Worst fitted lines (obs-calc/error):

    5:    2.1          7:    1.4          6:    1.3          1:   -1.1
   11:   -0.9         12:   -0.8          9:   -0.8         22:   -0.6
   23:    0.6         16:   -0.4         13:    0.4          2:   -0.4
   25:   -0.3         17:   -0.3         15:    0.3         21:    0.2
    8:    0.2         19:    0.1         10:   -0.1          4:    0.0
   18:    0.0         14:    0.0          3:    0.0         20:    0.0
   24:    0.0

    5:  2  1  2    1  1  1                    3824.5886   0.0206  0.010
    7:  7  3  5    7  1  6                    4100.8327   0.0138  0.010
    6:  2  1  2    1  0  1                    3913.2046   0.0135  0.010
```

```
   1:  5  2  3    5  1  4                    2569.4580  -0.0107  0.010
  11:  3  1  3    2  1  2                    5605.7733  -0.0091  0.010
  12:  3  0  3    2  0  2                    5619.5165  -0.0082  0.010
   9:  2  2  0    1  1  1                    5348.7281  -0.0078  0.010
  22:  4  0  4    3  0  3                    7358.9593  -0.0063  0.010
  23:  4  1  4    3  0  3                    7359.1292   0.0059  0.010
  16:  3  2  2    2  2  1                    6236.1417  -0.0043  0.010
-------------------------------------------------------------
```