A KNOWLEDGE-BASED SPECTROSCOPIC ASSIGNMENT SYSTEM

by

Jin Wang

TR97-112, April 1997

This is an unaltered version of the author's
MCS Thesis

Faculty of Computer Science
University of New Brunswick
Fredericton, N.B. E3B 5A3
Canada

Phone: (506) 453-4566
Fax: (506) 453-3566
E-mail: fcs@unb.ca
www: http://www.cs.unb.ca

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Jin Wang

B.Eng.(CS), Suzhou University, 1993

A Thesis Submitted in Partial Fulfillment of
the Requirements for the Degree of

Master of Science in Computer Science

in the Graduate Academic Unit of the Faculty of Computer Science

Supervisor(s):	B.G. Nickerson, Ph.D. the Faculty of Computer Science/Spatial Data Structures; Knowledge-Based Systems
	R.M. Lees, Ph.D. Physics Department/Microwave and Infrared Spectroscopy
Examining Board:	V.C. Bhavsar, Ph.D. the Faculty of Computer Science/Parallel Architectures and Algorithms; Learning Machines; Artificial Neural Networks; Multimedia; Computer Graphics; Digital VLSI systems, Chair
	D.M. Fellows, Ph.D. the Faculty of Computer Science/Simulation; Computer System Performance Evaluation; Operating and Distributed Systems.
	A.G. Adam, Ph.D. Chemistry Department/Experimental Physical Chemistry. Molecular Beams and Spectroscopy.

This thesis is accepted.

Dean of Graduate Studies

THE UNIVERSITY OF NEW BRUNSWICK

April, 1997 (of submission to Graduate School)

Abstract

Studying the energy level structure of different molecules by means of spectroscopy is one of the fields in physics and chemistry. MOSAA[1] developed in this thesis is a knowledge-based system which can assist researchers in the assignment of the peaks of the molecules in question by using the spectral information provided, along with a knowledge base containing known energy levels of the given molecules and spectroscopic assignment rules provided by physicists.

Rules together with their associated components (i.e. parameters, functions and properties) compose the knowledge base for methanol spectroscopy assignment. Rules and their components are written in plain text using special grammars. A compiler created using lex and yacc is used to translate a rule file into an internal knowledge base data structure. A total of 313 rules for spectroscopic assignment are defined.

The MOSAA system inference engine combines backward chaining and forward chaining as well as two special mechanisms 'TRY' and 'Restart'. This inference engine is written in C++, and was designed specifically to handle the "generate and test" process required for spectroscopic assignment.

An overview of the MOSAA implementation is given. This includes a description of the top level structure, preprocessing and user interface.

MOSAA was tested using two methanol species spectra (Spectrum $CH_3^{18}OH$ in the 900-1100 cm^{-1} region and Spectrum $CD_3^{16}OH$ in the 915-1030 cm^{-1} region). This testing showed that MOSAA successfully assigns 11 series in spectrum $CH_3^{18}OH$ testing and 11 series in spectrum $CD_3^{16}OH$ testing.

---

[1] MOlecular Spectroscopic Assignment Assistant

Acknowledgements

I would like to express my sincerely thanks to my supervisor Dr. B.G. Nickerson, for his tremendous encouragements, constant help, and inspiring guidance during the course of this project. Also, I would like to thank him for his patience and extra effort spending on correcting my language problems in my thesis writing.

Deep gratitude is due to my supervisor Dr. R.M. Lees who directed me into this special physics field which I had never been in before. His understanding and advice has always been a great help in my work.

I must say that, without my cousin Lihong, I would never have had the chance to start my study here. Without her support both academic and personal, this research could never have reached current achievements.

I want to say thanks to Anna, who has been taking care of me ever since I came to Canada.

Finally, I am deeply grateful to my family and friends for their love and continuing support. Specially, I want to show my thanks and love to my parents, they have been doing all they can for getting me better educations and better life.

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Chapter 1

Introduction

1.1 Problem definition

Studying the energy level structure of different molecules by means of spectroscopy is one of the fields in Physics and Chemistry.

Presently, the group of Dr. R.M.Lees of the Physics Dept. in the University of New Brunsick is focusing on studying the rotational and vibrational energy levels of methanol and its isotopic species [12,16,23,25,26].

Methanol, one of the simplest and most important molecules with hindered internal rotation, has received attention in Physics and Chemistry since early 1940 (Koehler and Dennison) [15].

The technique of high resolution infrared Fourier transform spectroscopy for studying the energy levels of methanol and its isotopic species, has had tremendous quantitative impact on molecular spectroscopy in the last decade [23]. The method involves first obtaining an infrared absorption spectrum (Fourier transform spectrum in a certain range and resolution) of the species of methanol being studied, which shows the transitions between the various energy levels of the molecule. The wavenumbers of the useful peaks of the absorption spectrum and their corresponding intensities are stored in a Peak Finder file. Then, using the current knowledge about energy level structures as well as a variety of analytical techniques, the peaks in the peakfinder file are labeled with the appropriate quantum numbers for the transitions. This leads to an understanding of the energy level structure and the internal interactions of the molecules.

The labeling process is called "energy level assignment". Fig.1.1 shows a piece of a spectrum, the corresponding part of the peak finder file, and the assigned labels.

Usually there are thousands of important peaks in one spectrum, especially in the high resolution case. Also, the spectra of methanol are highly congested, which makes doing the assignments by hand very time consuming.

The main emphasis of this thesis is on developing a knowledge-based system that can assist researchers in the assignment of the peaks of the molecules in question by using the spectral information provided and a knowledge base containing known energy levels of the given molecules and the rules provided by an expert for manipulating the information.

1.2 Knowledge-based systems

Begining in the mid sixties, expert systems expanded rapidly in many application areas such as chemistry, business, computer systems, and medicine [22].

Knowledge-Based systems are a generalization of expert systems that don't necessarily perform tasks at an expert level, but do utilize human knowledge in a form convenient for domain experts. Two basic components of a knowledge-based system are the knowledge base and inference engine.

The knowledge base contains the knowledge in a specific domain, while the inference engine controls the reasoning and has nothing to do with domain specific knowledge. This characteristic makes a knowledge-based system easier to maintain and expand since knowledge can be added or modified in the knowledge base. The inference engine is not affected by this knowledge modification process.

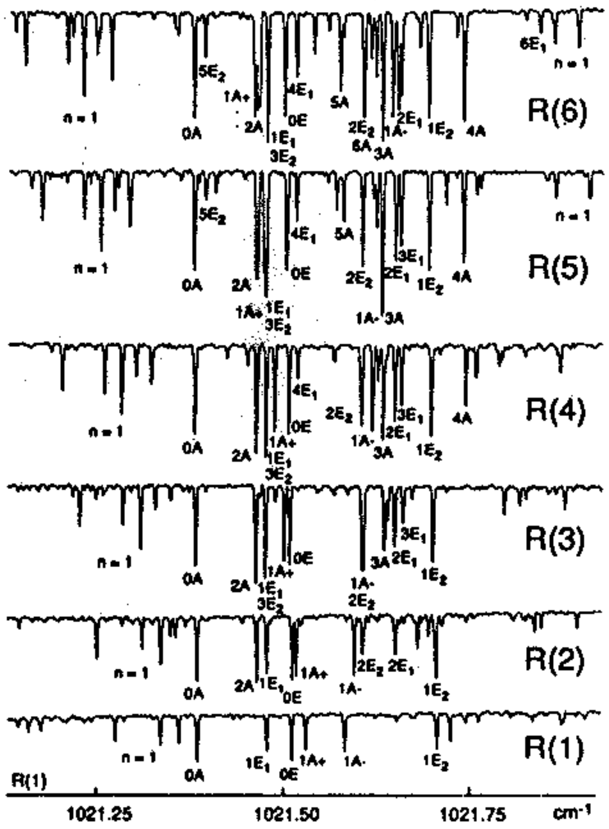


FIG. 1. Loomis–Wood diagram for the $R(0)$ to $R(5)$ $n=0$ multiplets in the R branch of the CO-stretching fundamental band of $^{13}CH_3OH$. Lines are labeled with their K values and torsional symmetries, and the $K=0A$ lines are aligned vertically. The wave number scale is shown at the bottom for the $R(0)$ multiplet. Torsionally excited $n=1$ series can be seen to the left and right of the diagram.

Peakfinder Output - C-13 Methanol - R(4) Multiplet		
Wavenumber (cm-1)	Intensity (Transm.)	Assignment P/Q/R(ntK,J)
1025.68067	0.9351	
1025.69544	0.7217	R(130,5) E
1025.75424	0.7055	R(121,5) E1
1025.77759	0.5811	R(122,5) A±
1025.79660	0.8047	R(123,5) E2
1025.81698	0.7671	R(125,5) A±
1025.87561	0.4620	R(010,4) A
1025.91770	0.9082	
1025.94533	0.8695	
1025.95745	0.3621	R(022,4) A±
1025.97041	0.3339	R(021,4) E1, R(023,4) E2
1025.98192	0.4822	R(031,4) A+
1026.00150	0.4703	R(030,4) E
1026.01313	0.7954	R(024,4) E1
1026.06334	0.8926	
1026.10190	0.5192	R(032) E2, R(110,7) A
1026.11675	0.4893	R(031,4) A-
1026.12408	0.7822	R(014,4) E2
1026.13114	0.4293	R(013,4) A±
1026.13528	0.9032	
1026.14645	0.5444	R(012,4) E1
1026.15568	0.6412	R(033,4) E1
1026.19519	0.4623	R(011,4) E2
1026.20665	0.9314	
1026.23985	0.6370	R(034,4) A±
1026.25270	0.7994	R(133,6) E1
1026.28286	0.8626	
1026.28712	0.8993	R(137,8) A±
1026.31775	0.9179	
1026.35974	0.9222	
1026.36342	0.8256	R(132,5) E2
1026.42202	0.7769	R(111,8) E2

Figure 1.1: Part of the R-Branch of the CO-Stretching Band of C-13 Methanol, with Peakfinder Output and Partial Assignments in the R(4) Multiplet Region (from [16]).

The architecture of a simple knowledge-based system is shown in Fig 1.2.

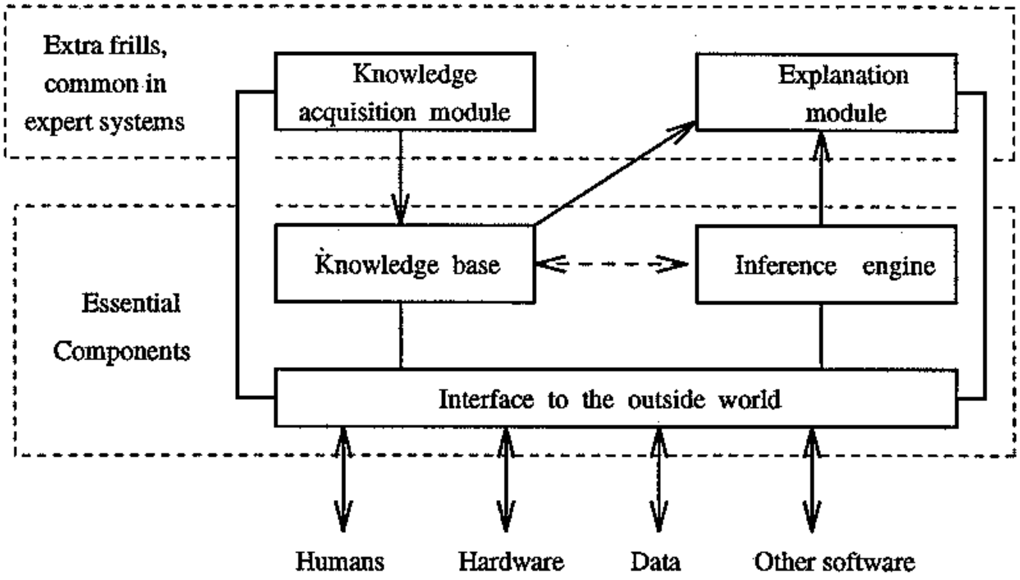


Figure 1.2: The architecture of a simple knowledge based system (from [14] (KBS)).

Knowledge bases can be complex depending on the form of knowledge required. The simplest knowledge base contains rules and facts. Transferring the knowledge into rules and facts is an important part of knowledge based systems called knowledge representation. Rules usually have the style:

label	**IF**	$\mathit{condition}_1$ $\mathit{condition}_2$ ... $\mathit{condition}_n$	Premise
	THEN	conclu_1 conclu_2 ... conclu_n	Conclusion

Inference engines can operate in different ways due to the corresponding control needed for dealing with the different knowledge and tasks. Two major types of inference engine are forward-chaining and backward-chaining. Forward-chaining is a data driven approach while backward-chaining is a goal driven approach.

1.2.1 DENDRAL

DENDRAL is the first large-scale program to embody the strategy of using detailed, task-specific knowledge about the problem domain as a source of heuristics [9,10, 11]. DENDRAL is not a simple program; it includes two subsystems called Heuristic DENDRAL and Meta-DENDRAL. Meta-DENDRAL is a learning system which belongs to the field of knowledge acquisition, thus here we won't give further discussion about this.

Heuristic DENDRAL is a system that incorporates specific knowledge of chemistry and mass spectrometry, accepts a mass spectrum and other experimental data from an unknown compound as input, and produces an ordered set of chemical structure descriptions hypothesized to explain the data. The basic method used is the generate-plan-test paradigm [11].

"Generator" is a program that enumerates for a particular problem its potential solutions, which are expressed as chemical graphs in the case of DENDRAL [11].

"Planner" employs task-specific knowledge, which includes mass spectrum and planning rules to find constraints for the generator. Further selection of the set of solutions produced by "generator" is performed by a third stage, the "test" [11].

The tester incorporates a theory of mass spectrometry that predicts what fragmentation a proposed chemical structure will undergo in a mass spectrometer and constructs a mass spectrum accordingly. This predicted spectrum may then be compared to the one produced in the laboratory [11].

The inference engine used in DENDRAL is forward chaining. A sample rule used in DENDRAL is shown in Fig 1.3.

1.2.2 MYCIN

MYCIN is a rule-based expert system, developed for diagnosis of infectious diseases in medicine. MYCIN uses a goal driven backward chaining inference engine. The goal

```
If the spectrum for the molecule has two peaks at masses x1 and x2
   such that
   1. x1 + x2 = M + 28
   2. x1 - 28 is a high peak, and
   3. x2 - 28 is a high peak, and
   4. at least one of x1 or x2 is high
Then the molecule contains a ketone group
```

Figure 1.3: A sample rule in DENDRAL.

rule starts the whole session by determining if there is an organism requiring therapy. A sample rule is as shown in Fig 1.4

```
IF  1) The culture was taken from a sterile source, and
    2) It is definite that the identity of the organism
       is one of:  staphylococcus-coag-neg bacillussubtilis
       corynebacterium-non-diphtheriae
THEN:
       There is strongly suggestive evidence (.8) that the
       organism is a contaminant.
```

Figure 1.4: A sample rule in MYCIN

MYCIN has a powerful consultation and explanation facility associated with the main inference engine. Uncertainty is also used in MYCIN which enhances its performance [20].

1.2.3 TI PC Easy

TI PC Easy is an expert system shell that can be used to build a knowledge based system. There are some good characteristics in the structure of the knowledge base that were derived from MYCIN. The inference engine of PC Easy has combined forward chaining and backward chaining which is different from traditional inference engines as in DENDRAL and MYCIN.

The characteristics of TI PC Easy contributed to the ideas used in developing the knowledge based system in this thesis.

There are three basic components in the PC Easy knowledge base: properties, parameters and rules. The reference guide of PC Easy [21] gives the definitions of these components:

1. **properties**

   A knowledge base property is a structure that contains a piece of information about the knowledge base as a whole or controls a knowledge base characteristic. For example, the property INITIALDATA tells PC Easy what information to prompt a client for at the start of a consultation.

2. **parameters**

   A parameter is a structure that identifies or contains a piece of information that PC Easy uses to arrive at a conclusion. For example, the parameter TEMPERATURE might contain a piece of information about the weather.

   A certainty factor can be used to indicate a measure of confidence in the value of a parameter.

   Parameters can have properties associated with them.

3. **rules**

   With parameters and knowledge base properties, rules are one of the three basic knowledge base components. PC Easy rules are if-then statements that express the relationships among parameters. You write PC Easy rules in a language similar to English.

   Rules in PC Easy are written in Abbreviated Rule Language (ARL), which combines parameter names and values with ARL functions.

   Like parameters, rules also can have properties associated with them.

A sample rule used in PC Easy is shown in Fig 1.5.

```
IF      (CREDIT = GOOD AND LOAN-DESIRED < 10000)
     OR (SAVINGS = SUBSTANTIAL AND SALARY = HIGH-RANGE)
THEN    LOAN = APPROVED
```

Figure 1.5: A sample rule in PC Easy.

A PC Easy rule can be a consequent rule or antecedent rule according to its properties associated with the rule. Antecedent rules are used in forward chaining and consequence rules are used in backward chaining.

As discussed in the PC Easy reference guide [21], antecedent rules differ from consequence rules in three major ways:

- PC Easy tries an antecedent rule after it determines the value for a parameter in the IF statement of that rule. PC Easy tries a consequence rule if the rule's THEN statement assigns a value to a parameter that PC Easy needs.
- If another parameter in the antecedent rule's IF statement lacks a value, PC Easy does *not* try to determine that value.
- PC Easy tries an antecedent rule each time it determines a value for one of the parameters in the rule's IF statement. PC Easy tries a consequence rule only once.

1.2.4 Knowledge-based systems used in spectroscopy

Several knowledge-based systems have been developed for use in physics and chemistry spectroscopy after DENDRAL.

As we know, DENDRAL is used in organic chemistry and uses the *generate*, *plan* and *test* approach to identify unknown compounds using mass spectroscopy. Most of the recent knowledge based systems in spectroscopy are used in identifying and interpreting the structure of compounds with corresponding spectra.

One project which has several papers appearing in recent years is **ESSESA: an expert system for structure elucidation from spectra**. This project uses a knowledge-based system for the analysis and the interpretation of NMR spectra such as ^{13}C-NMR [1] and ^{1}H-NMR [3].

EXPIRS is a heuristic knowledge-based system which is used for infrared spectra interpretation. This program generates alternative substructure sets, based on a hierarchical organization of the knowledge base, utilization of molecular formula, and a more precise subroutine for selection of the substructures [2].

SCANNET is a system applied to qualitative analysis of organic substances, i.e. in identification of the structure of a given (unknown) compound. The main feature of the system is the simultaneous access to more than one database and also simultaneous display (on one screen) of up to six different (^{13}C-NMR, ^{1}H-NMR, IR, MS, RA and UV) spectral curves for profound and advanced interpretation [6].

HEPHESTUS is an expert system implemented in a PROLOG environment, for the interpretation of pyrolysis mass spectra (PyMS) of three categories of polymers: polyesters, polyethers and polyureas. The knowledge of the domain is organized in the form of rules that relate polymer structures with mass spectra characteristics. The IF part of the rules test for matching the information extracted from the unknown PyMS spectra with those of the knowledge base. The knowledge base is organized as a dendrite, i.e., the polymer structures are organized hierarchically as a tree [4].

Some other systems are not used in identifying and interpreting the structure of the compounds with corresponding spectra.

One expert system (ES) was built to allow inexpert users to interpret infrared spectra in a few minutes. The ES contains a knowledge base which is structured following logical representation schemes, and the inference process is carried out by operating on rules and principles. In order to use the ES, users must feed the spectrum peak frequencies to the system, then the ES inference process begins and the ES output interface suggests the possible functional groups present in the sample [5].

So far, there is no knowledge-based system found that assists with methanol spectroscopic assignment.

1.3 Scope of thesis

This thesis mainly discusses the method used in methanol spectroscopic assignment knowledge representation and the implementation of MOSAA[1], which assists physicists in methanol spectroscopic assignment.

After the brief introduction and literature review of knowledge-based systems given in the present chapter, chapter 2 outlines the essential background concepts in methanol spectroscopic assignment used by R.M.Lees' group. A literature review of previous computer programs developed for assisting methanol spectroscopic assignment is also given in this chapter.

Chapter 3 deals with design of this methanol spectroscopic assignment assist system. Knowledge representation of Methanol spectroscopic assignment is introduced. Rules as well as the components associated with them are also presented to describe the way of translating methanol spectroscopic assignment knowledge into the MOSAA knowledge base.

An important part of MOSAA is the Inference Engine. Chapter 4 discusses its structure, functions and the way it is implemented.

Chapter 5 continues discussing the implementation of some other parts in MOSAA. It includes the internal data structures, preprocessing, user interface and explanation facility.

Chapter 6 describes the processes used in testing MOSAA and the corresponding results of the testing.

---

[1] MOlecular Spectroscopic Assignment Assistant

The last chapter gives conclusions and discusses the work to be done in the future.

Further specific details on MOSAA are contained in the MOSAA developer's guide[13].

Chapter 2

Methanol Spectroscopic Assignment

This chapter describes the physical and chemical problems addressed by this thesis. In order to understand the research presented here, it is necessary to introduce some elementary concepts about methanol spectroscopic assignment.

The energy level structure of the methanol molecule is what we are interested in. Energy levels are quantized. When the molecule absorbs energy equal to the change in energy, ΔE, between two energy levels, the molecule jumps to the higher energy level as shown in Fig 2.1. This is called a transition.

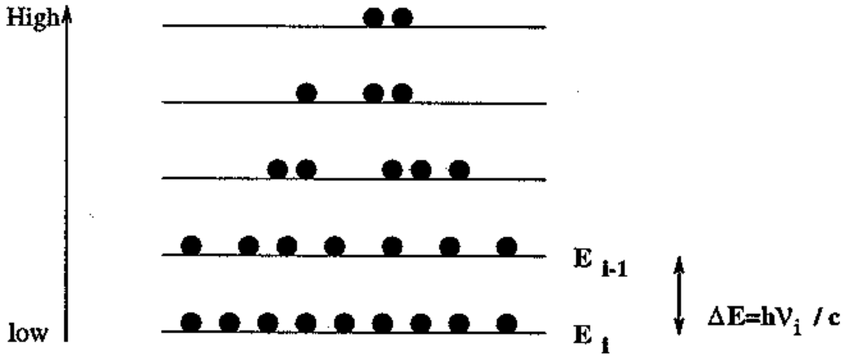
The number of molecules, n, existing in any particular energy level decreases exponentially as you go higher in energy. So this can be calculated as $n \propto e^{-E_i/(kT)}$, where E_i is the energy of an energy level, i; k is the Boltzmann constant; and T is the temperature of the sample, in Kelvin.

One can study the energy levels of the methanol molecules by investigating the methanol spectrum, which shows the energy level transitions of molecules.

The x-axis used for the spectrum is wavenumber, in units of cm^{-1}, instead of frequency. Wavenumber and frequency have the relationship:

$$wavenumber(cm^{-1})/frequency(MHz) = 1/29979.2458(s/cm). \tag{2.1}$$

The symbol ν_i is used to denote the wavenumber in the following sections.



Molecular distribution: $n \sim e^{-E/kT}$
h -- planck's constant
c -- speed of light

Figure 2.1: Quantized energy levels of methanol molecules.

Fig 2.2 shows the method used to produce a methanol spectrum. Light (normally infrared (IR) or far-infrared (FIR)) containing a range of wavenumbers ν_n passes through an absorption cell full of methanol vapour. As shown in Fig 2.1, when a wavenumber ν_i equals the ΔE of two energy levels, it is absorbed, and an energy level transition occurs. Therefore, the intensity of the light with wavenumber ν_i decreases.

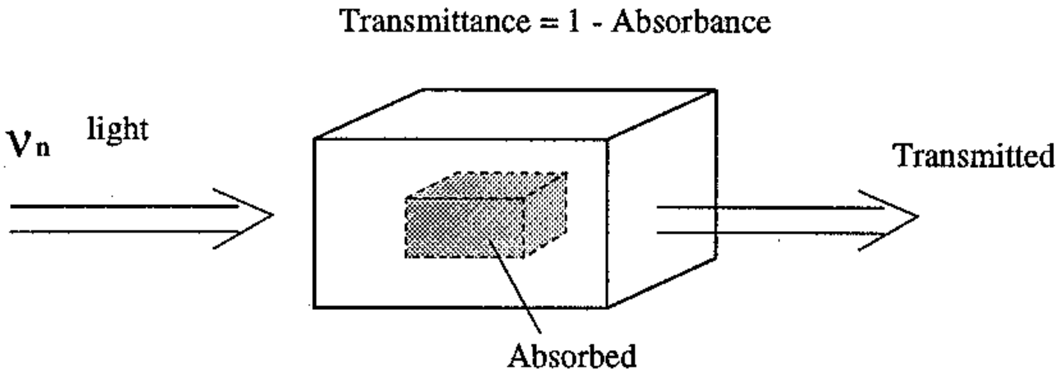


Figure 2.2: Transmitting light through a gas cube full of methanol.

If there is no gas inside the cell, there is no absorption and there is a flat spectrum with 100% transmittance of the light as shown in Fig 2.3(a).

With gas in the cell, absorption occurs at all of the possible ν_i transition wavenumbers, and a spectrum is observed as shown in Fig 2.3(b).

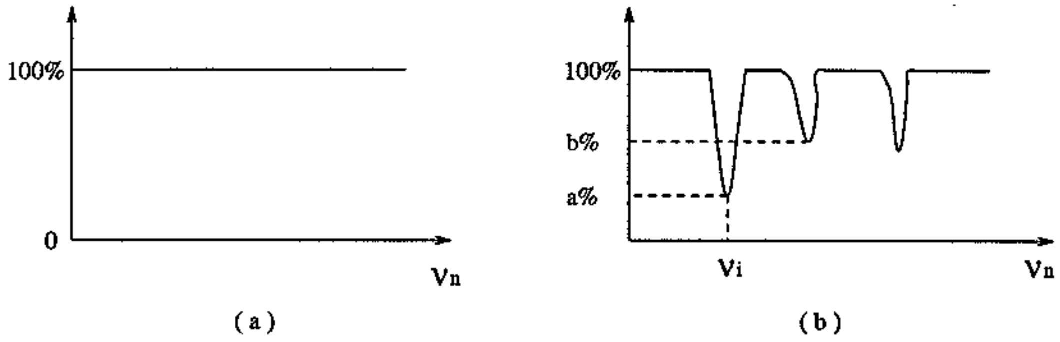


Figure 2.3: Spectra for (a) is empty, and (b) cell containing an absorbing gas showing absorbing transitions at wavenumber ν_i.

If the intensity at wavenumber ν_i in light transmitted through the cell is a, which means the transmittance is a, then the absorption is 1-a. Therefore, by using an absorption spectrum, we can study the energy level structure of methanol molecules.

2.1 The structure of the CH_3OH spectrum

2.1.1 Methanol energy levels and transitions

The total energy levels of a molecule are determined by its vibrational, internal rotational (torsional) and rotational states as:

$$E_{total} = E_{vib} + E_{tor} + E_{rot} \tag{2.2}$$

where E_{vib} - net energy in the 11 small-amplitude vibrations

E_{tor} - internal rotation (torsion) energy

E_{rot} - rotational (overall) energy

Methanol has a total of 12 normal fundamental vibrational modes, as indicated in Fig 2.4 [23].

When $E_{vib} = 0$, the energy level is called "the vibrational ground state".

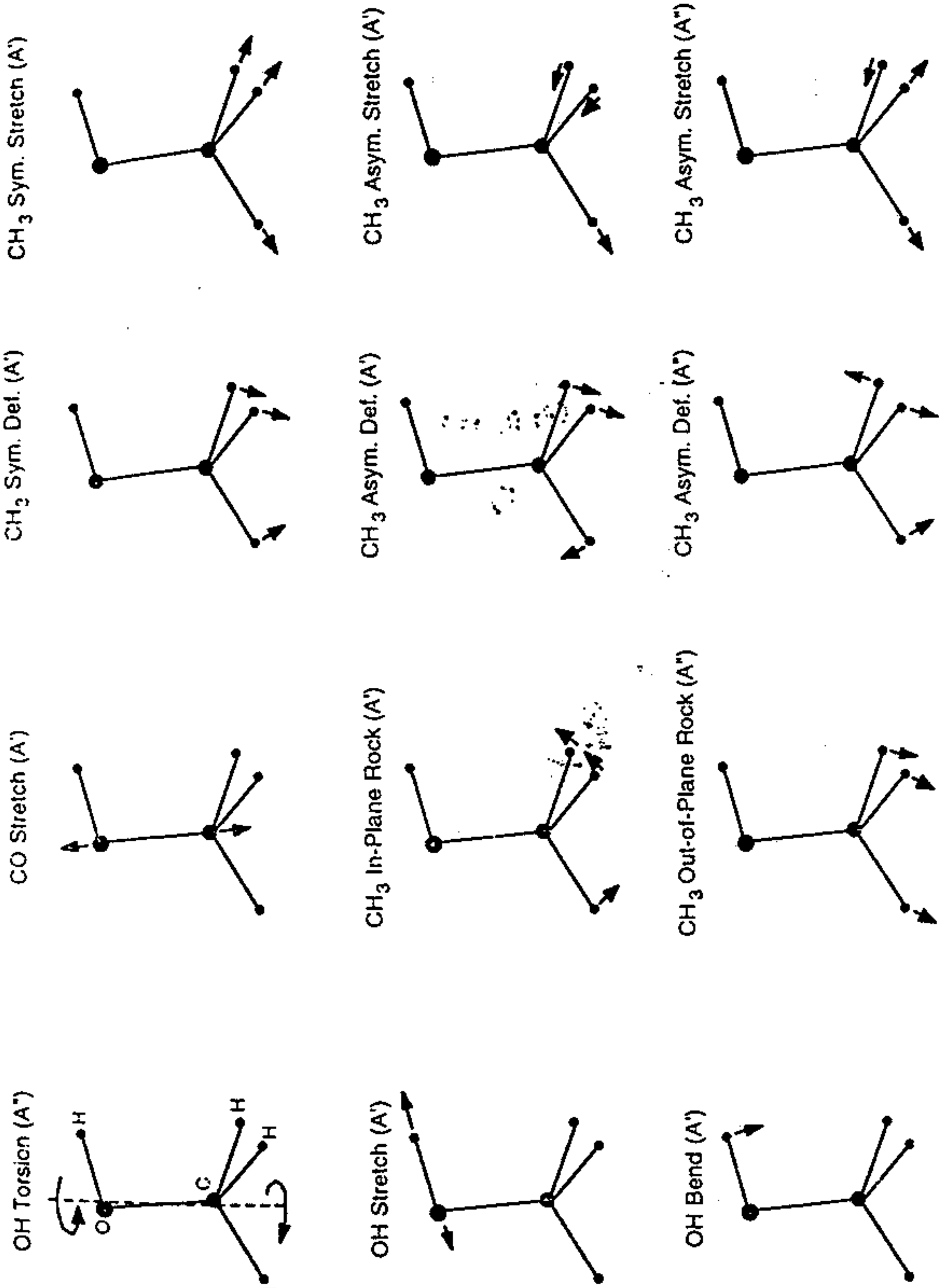


Figure 2.4: Schematic representations of the 12 fundamental vibrational modes (11 small amplitude vibration and one torsion) of methanol (from [23]).

To represent the energy levels' transitions, the following symbols are used:

$(V_t T_s K, J)^{V_{vib}}$ or $(n\tau K, J)^{V_{vib}}$

where

$\mathbf{V_{vib}}$ determines the upper vibrational state. Therefore, V_o represents the ground state, and V_{co} represents the CO stretching state. V_{vib} can have values 0, 1, 2 ..., e.g.

$V_{co} = 0, 1, 2 \ldots$
0 - ground state
1 - first vibrational excited state
2 - second vibrational excited state

$\mathbf{T_s}$ and τ determines the internal rotation (torsional) state. T_s represents the torsional symmetry, which can be A, E_1, or E_2. Another symbol which often used instead of T_s is τ which has value 1,2 or 3.

$\mathbf{V_t}$ (or n) can be 0, 1, 2, 3, ..., which represents the ground torsional state, first excited torsional state, etc.

J is the total rotational angular momentum. K is the component of J along the z-axis. We have:

J = 0, 1, 2, 3 ...
K = 0, 1, 2, ... J

Once we have these symbols, the energy level of a molecule can be written using the energy expansion model [16] as follows:

$$\begin{aligned} E(n\tau K, J)^V &= E^V_{vib} + W^V(n\tau K) + B^V(n\tau K)J(J+1) - \\ &\quad D^V(n\tau K)J^2(J+1)^2 + H^V(n\tau K)J^3(J+1)^3 + \\ &\quad \text{(asymmetry splitting term)} \end{aligned} \tag{2.3}$$

where V denotes the vibrational state of energy E^v_{vib}, W is the J-independent part of the torsion-rotation energy, and B, D and H are effective state-dependent molecular parameters. Although the variations with (n τ K) of the latter are small, they are clearly resolvable with the present FTIR[1] measurement accuracy. Since the B^o and D^o values can also be calculated with some confidence for the ground vibrational state, they furnish a valuable assignment tool [16].

---

[1] Fourier Transform InfraRed

2.1.2 R, P, Q branches

Each mode in Fig 2.4 represents a band in the methanol spectrum. A band usually falls in a certain range of the spectrum, but the regions for two or more bands may overlap.

The lines corresponding to high absorption in each band are grouped into branches labeled as P, Q and R, for ΔJ = -1, 0 and +1 transitions, respectively, as shown in Fig 2.5.

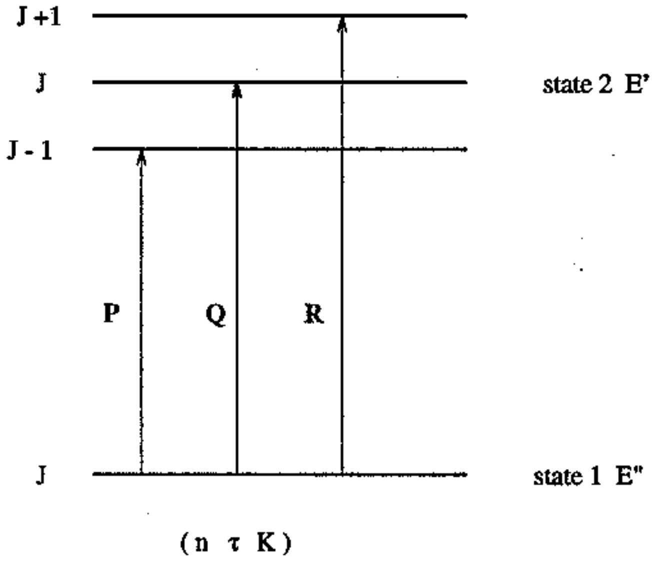


Figure 2.5: Transitions in R, P, Q branches.

Fig 2.6 is a spectrum of the CO stretching band of CD_3OH. In the low resolution spectrum, there is a very clear P, Q and R branch pattern. The P and R branches show very clear multiplets of lines; the Q branch is highly congested and doesn't show clear multiplets. Diagram b) is a section of the high resolution spectrum containing the P(19) multiplet, which appears as a single line in the low resolution spectrum. Lines in the same multiplet have the same J value; (e.g. 19 in P(19) represents the lower-state J value for this multiplet) but different (n τ K) values. If we select the line with the same (n τ K) value from each multiplet, they build a pattern similar to the diagram that shown in Fig 2.6 (a). These lines with the same (n τ K) value but

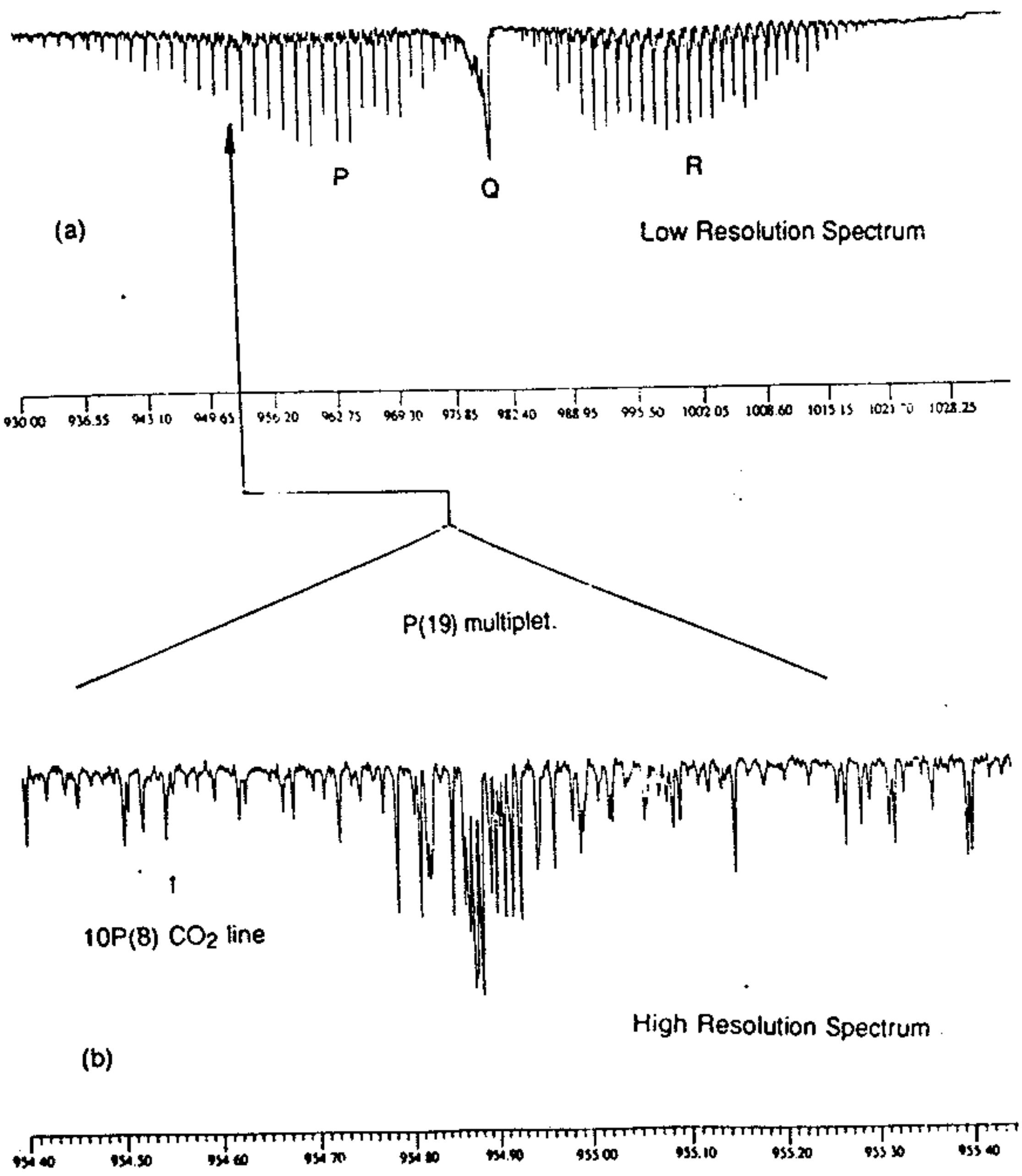


Figure 2.6: (a) Low resolution spectrum of CD_3OH in the 930-1030 cm^{-1} region; (b) 0.002 cm^{-1} high resolution spectrum of the P(19) multiplet (from [23]).

different J values in the IR [2] spectrum belong to one group: a “series”.

Lines in the P branch or R branch have smaller J values when they are closer to the Q branch. The wavenumbers can be expressed according to equation 2.3 and Fig 2.5 with the energies expanded in powers of J(J+1). If the small D and H terms are ignored, since B'' and B' are very close, we get the following equations:

$$R(J) = E'(J+1) - E''(J) \approx E^{V}_{Vib} + 2B''(J+1) \tag{2.4}$$

and

$$R(J) - R(J-1) = 2B'' \tag{2.5}$$

Thus, the distance between two neighboring lines in the R branch of the same series is close to a constant in the case of low J. The P branch has similar behaviour. For the Q branch, we can’t ignore the difference between B' and B'' and we get

$$Q(J) - Q(J-1) \approx 2(B' - B'') \tag{2.6}$$

Since $(B' - B'')$ is very small, the distance between two Q lines turns out to be small, which causes the highly congested appearance without multiplets in the Q branch.

2.2 Difference table spreadsheets

As mentioned in 1.1, once an absorption spectrum and its corresponding peak finder file have been obtained, then by using the current knowledge about the energy level structures as well as a variety of analytical techniques, peaks in the peakfinder file can be labeled with the appropriate quantum numbers for the transitions.

Due to the congestion of lines in the spectrum, we assign one series at a time. One technique used for initial sorting of the series and the following assignment of the series is using difference table spreadsheets.

---

[2] InfraRed

Table 2.1 shows a part of a difference table spreadsheet.

Table 2.1: A sample section of a difference table spreadsheet (Note that the Q branch is missing from this table due to space restrictions).

	R Branch	[Series 1]				P Branch	
J	R(J)	Δ1	Δ2	Intensity	J	P(J)	Δ1
4	1015.573578	1.444535		0.7245	4	1000.194709	-1.630461
5	1017.018113	1.427566	-0.016969	0.5955	5	988.564248	-1.646984
6	1018.445679	1.410012	-0.017554	0.4666	6	996.917264	-1.663689
7	1019.855691	1.393535	-0.016477	0.4017	7	993.573300	-1.680275
8	1021.249226	1.376004	-0.017531	0.2994	8	991.876305	-1.696995
9	1022.625230	1.358654	-0.017350	0.3554	9	990.162255	-1.714050
10	1023.983884	1.341201	-0.017453	0.3373	10	991.876305	-1.714050
11	1025.325085	1.324044	-0.017157	0.1976	11	990.162255	-1.729513

The basic part for each sub-branch in the spreadsheet has 5 columns for each line: the J value, the wavenumber, first difference, second difference and line intensity. The first and second differences are defined as $\Delta 1(J) = \nu(J+1) - \nu(J)$ and $\Delta 2(J) = \Delta 1(J) - \Delta 1(J-1)$.

From the discussion in section 2.1.2, the relationships between Δ1, Δ2, ΔB and J can be expressed as [25]:

R branch: $\Delta 1(J) = R(J+1) - R(J) = 2\ \Delta B(J+2) + 2B''$, $\Delta 2 = 2\Delta B$
P branch: $\Delta 1(J) = P(J-1) - P(J) = 2\ \Delta BJ - 2B''$, $\Delta 2 = 2\Delta B$
Q branch: $\Delta 1(J) = Q(J+1) - Q(J) = 2\ \Delta B(J+1)$, $\Delta 2 = 2\Delta B$

Normally lines belonging to the same series have second differences Δ2 which normally follow a smooth trend [25].

For different bands, ΔB will be different due to changes in B'; therefore the Δ2 values for each band are different. For example, for the CO stretching fundamental $\Delta 2 \approx -0.016cm^{-1}$, while for the CH_3 in-plane-rocking fundamental $\Delta 2 \approx -0.006cm^{-1}$ [25].

For the R branch, $\Delta 1 \approx 2B''$ decreases when J increases. $\Delta 1 \approx -2B''$ for the P branch, and increases when J increases. Δ1 is negative for the Q branch and increases with J.

In the case of low J, the J value of a line with wavenumber ν_i usually can be determined by

$$J \approx (\nu_i - \nu_{Q(0)})/2B'' \tag{2.7}$$

where Q(0) is the origin of the Q branch.

2.3 Basic methanol spectroscopic assignment techniques

To assign a new spectrum, one way to get started is to find three neighboring lines in one series first, and then expand to get the whole series. This process is repeated, each time assigning one series.

Fig 2.7 shows a typical structure for three neighboring multiplets. These are not from a real spectrum but are just used here to explain what we call "Three Line Group".

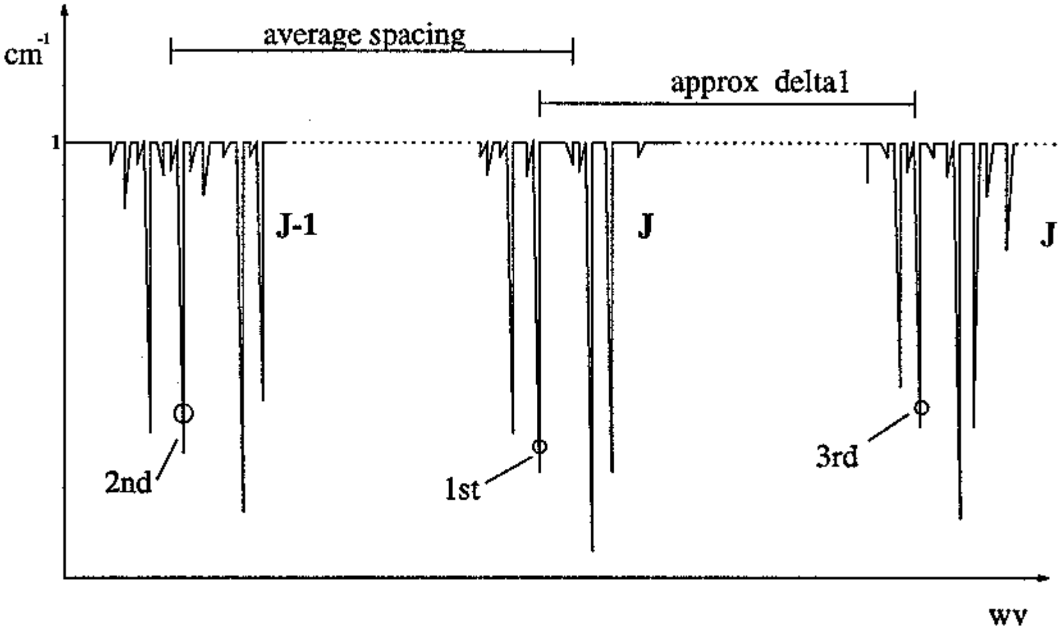


Figure 2.7: A sample figure to explain the "Three Line Group".

The first line can be randomly picked from a low J but sufficiently strong multiplet. The second line is picked in a multiplet next to the first one, which can be either the J-1 multiplet as shown in Fig 2.7, or the J+1 multiplet. To pick the second line, one needs to know the approximate average spacing between two multiplets, which is usually close to $2B''$ in the low J case [3]. The intensity of the second line in principle should be close to the intensity of the first line, except in the case of overlapping[4]. Overlapping is a complication which leads to difficulties in performing the assignment.

The data of the first line and the second line are put in the spreadsheet which is ready for searching for the third line, as shown in Fig 2.8.

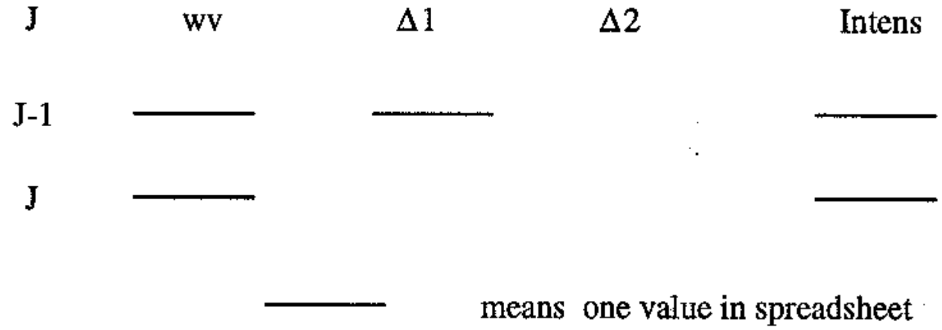


Figure 2.8: Two lines found.

We then use Δ1 as a trial spacing to search for a third line and get the spreadsheet of Fig 2.9, which is the base for expanding to the other lines in one series.

As mentioned in section 2.2, Δ2 is close to a constant. Thus, to search for the (J-2) and (J+2) lines, we have:

$$\begin{aligned}\nu_{J-2} &= \nu_{J-1} - \Delta 1_{J-1} + \Delta 2_J \\ \nu_{J+2} &= \nu_{J+1} - \Delta 1_J + \Delta 2_J\end{aligned}$$

---

[3] When the R,P,Q pattern is clear, there are clear multiplets; otherwise, we don't have clear multiplets, but the approximate spacing between the first line and second line is still close to $2B''$.

[4] When two or more lines are too close in a spectrum, they appear as one line in the peakfinder file with greater intensity.

J	wv	Δ1	Δ2	Intens
J-1	———	———		———
J	———	———	———	———
J+1	———			———

——— means one value in spreadsheet

Figure 2.9: Three lines found.

During this expansion, the main problem one has to deal with is the overlap case which alters the expected values for the wavenumber shift and intensity.

The expansion is continued as far as possible. It will finally stop due to one of the following reasons: (a) in the search direction towards the Q branch, the leftmost line has a J value equal to K for the R branch (or the rightmost line has a J value equal to K+1 for the P branch); (b) in the search direction away from the Q branch, lines become weak and no longer appear in the Peakfinder file, hence we don't need to search anymore; (c) an expected line is missing in the Peakfinder file; (d) overlap causes a shift in the expected line; (e) a line is perturbed; (f) there was a mistake in picking previous lines, and some other cases.

If we get a significant number of consistent lines, we assume that this IS a series. The J value of a low J line then will be determined by equation 2.7 and can be expanded to all the other lines.

The series we get must belong to one branch. If this is the R branch, say (the P branch is just the inverse case), the next step is to try to find corresponding lines in the P branch using known ground state data and the existing R branch lines and doing an expansion in the P branch; then coming back to get more lines in the R branch from the existing lines in the P branch. During this process, the Q branch lines (if this series has a Q branch) are also searched.

As Fig 2.10 shows, ground state combination differences are used for the $R \to P$ search[5] and the inverse $P \to R$ search[6].

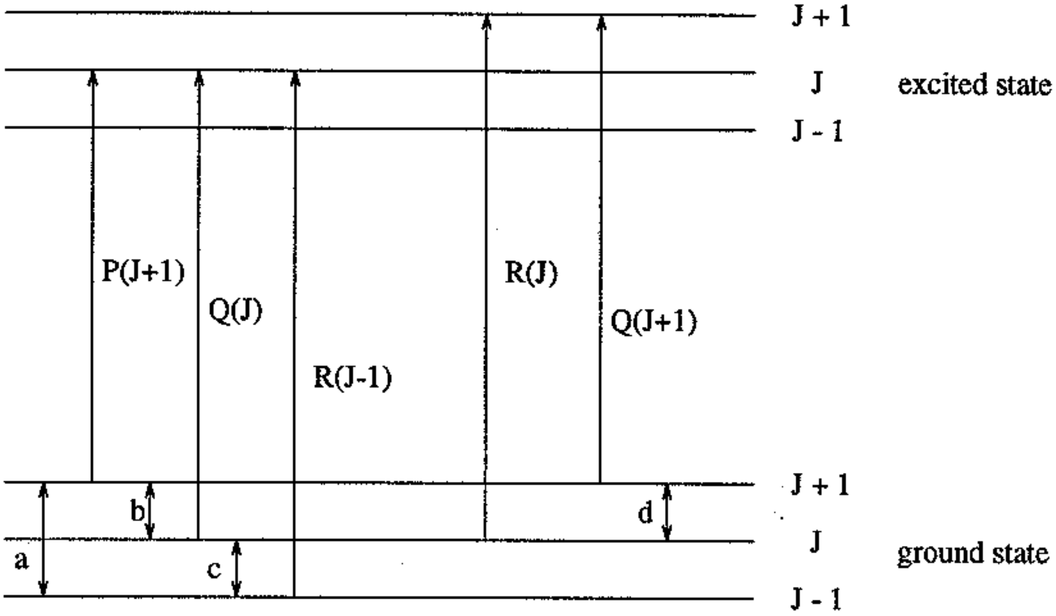


Figure 2.10: Combination differences and combination loops.

In Fig 2.10, "a" is the R-P combination difference,

CD(J-1)=R(J-1) - P(J+1)= a = b+c= E"(J+1) - E"(J-1)

The combination differences for each series are determined in two ways; i.e. (a) from previous FIR or IR spectroscopic measurements, or (b) by calculation of the ground state energies. Once we have R(J-1), we can get P(J+1) as:

$$P(J+1) = R(J-1) - a \tag{2.8}$$

Since there may be systematic errors in the combination differences, especially in the calculated combination differences, the P lines obtained in this way are not very

---

[5] Search P branch of current series using already found lines in R branch.

[6] Search R branch of current series using already found lines in P branch.

accurate. Thus techniques and pratical experience must often be used to determine the right P line in the Peakfinder file.

The technique of "combination difference loops" is used to try to confirm the relationship between the selected related R,P,Q lines. From Fig 2.10 we have the following equations:

$$\begin{aligned} R(J) - Q(J+1) &= d \\ Q(J) - P(J+1) &= b \end{aligned} \tag{2.9}$$

Since b=d, when the lines we select satisfy this relationship (to within the experimental uncertainty), these lines are confirmed.

By using the combination differences, we transfer the "Three Line Group" plus one higher or lower line from the R branch to the P branch first. When these lines are confirmed, we have a high confidence in saying that the "Three Line Group" and the combination difference series chosen are right. At this point, (n τ K) is identified from our combination difference data base.

The Lines in the P branch are then expanded as much as possible. When the expansion gets stuck, P → R transfer starts. By doing this $R \rightarrow P$ and $P \rightarrow R$ back and forth searching, more and more lines are identified until no more new lines can be found.

Solution of the problems due to overlap, perturbation, missing lines, imprecise CD's and other situations is fairly complicated and depends heavily on the experience of the spectroscopic assignment expert. The complete details are not covered here.

2.4 Existing programs for assisting spectroscopic assignments

To assist physicists doing methanol spectroscopic assignments, several computer programs have been developed. Two of the methanol spectroscopic assignment computer programs are introduced here.

2.4.1 Ritz

The *Ritz* program was developed by Dr G. Moruzzi at the University of Pisa using Gnu C in DOS. It has several modules including line assignment, fitting, etc.

This program uses existing assignments as well as the Hamiltonian technique. If we already know several lines in one series, such as R(2), R(4), R(5)...., the constants B, D... in equation 2.2 can be deduced by fitting. Thus, the other lines in this series can be determined approximately by using this equation with the known constants.

In Fig 2.11, each dot represents a set of the energy levels with the same (n, K) but different J. Transitions A, B and C represent FIR energy level transitions, since they change the K value. Once we know these transitions, transition D can be derived and confirmed.

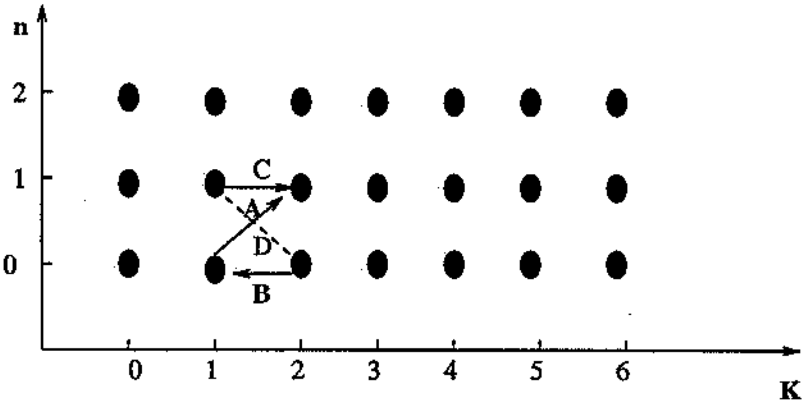


Figure 2.11: Energy level transitions.

These are the basic ideas and techniques used in the *Ritz* program.

2.4.2 Giessen LOOMIS-WOOD

The *Giessen LOOMIS-WOOD* program was developed at the Justus Liebig University, Giessen, Germany.

As introduced in the manual of this program [17], the principle of the LOOMIS-WOOD program was first suggested by Loomis and Wood in 1928 [17]. The program cuts the spectrum into segments of 2B, where B is the rotational constant. The intensities of the lines are represented by the heights of triangles plotted on the screen. With a suitable value of B, lines belonging to one series will appear as a vertical line or at least as a recognizable curve, and can be assigned as a set of transitions having the same values of all quantum numbers except J. Lines belonging to one series can be recognized, tagged and written into a specified file. To compensate for the convergence of the spacing in the R branch and the divergence in the P branch, due to the inequality of B'' and B', the starting wavenumber of the next row is not equal to the last wavenumber of the current row. It is corrected, so that the peaks of a series for which the constants are known appear as a truly vertical line.

The method of combination differences (CD) may be used to assign a series which shares a common lower vibrational level with a well-known series. The differences in wavenumber between transitions with a common lower state depend only on the properties of the upper vibrational states. The method can be used to identify one branch if you know the other one, or to confirm J's if B'' is already known.

This program is implemented using the Pascal language on a PC.

Chapter 3

System design

3.1 Methanol Spectroscopy Assignment Knowledge Representation

As mentioned previously, MOSAA[1] developed in this thesis is a knowledge-based system which can assist researchers in the assignment of the peaks of the molecules in question by using the spectral information provided and a knowledge base containing known energy levels of the given molecules and the rules provided by the experts for manipulating the information.

Knowledge representation is the basic and key part in system design. Only when the method of transferring the knowledge of spectroscopic assignment has been settled, can the knowledge-based system main components (i.e. knowledge base and inference engine) be designed and implemented.

Rules together with their associated components (i.e. parameters, functions and properties) compose the knowledge base which contains methanol spectroscopy assignment knowledge in this thesis. The complete context-free rule grammar for MOSAA is given in Appendix A.

---

[1] MOlecular Spectroscopic Assignment Assistant

3.2 Parameters

Parameters are one of the most important concepts in the MOSAA system. A parameter is a structure that identifies or contains a piece of information that the inference engine uses to arrive at a conclusion [21].

Most parameters in the MOSAA knowledge base have a physical meaning in methanol spectroscopic assignment. In this sense, parameters can be roughly classified into three groups:

1. Parameters represent terms people use in methanol spectroscopic assignment. For example:

   `Fir_L_S_idx` refers to the first line of "Three Line Group" in the current series as introduced in section 2.3.

   `Cur_Series.n`, `Cur_Series.t`, `Cur_Series.K` and `Cur_Series.Symm` represent (n τ K) and Symmetry of the current assigning series as introduced in section 2.1.1.

   More of these kinds of parameters are explained later in this section.

2. Parameters are used for referring to some steps in the process of doing an assignment. For example:

   When parameter `Sec_L_Found` equals 1, this means the second line in the current assigning series has been found.

   When parameter `P_Initial_Assign` is set to 1, the P initial assignment (First time $R \rightarrow P$ and P extension) introduced in section 2.3 has been done.

3. Parameters are used to enable easy rule writing and for overall connecting and consistency purposes. These are defined to assist in guiding the running of the inference engine. Some examples are:

Parameter `TEMPI1` is used for reserving an integer value temporarily. The scope of these "Temp" parameters is just within the current rule.

Parameters `L1`, `L2`, …are used for the `Match` *Property* which is described in section 3.4.

A Parameter also can appear as one of the following types in a rule:

Simple Parm -

Plain identifier; e.g.

`Pro_L, Fir_L_S_idx, TEMPI1`

Index Parm -

Plain identifier associated with an extra index; e.g.

`Cur_CD[0], Cur_CD[8]` …

This kind of parameter is not currently used (even `Cur_CD[0]` is shown here only as example). The rule base is still under construction, and this parameter type is kept for later convenience.

Field Parm -

Plain identifier associated with fields; e.g.

`Cur_Series.K, Cur_Series.Symm` …

Index_Field Parm -

Identifier associated with index and fields; e.g.

`Cur_R_Peaks[14].wv, Cur_P_Peaks[0].intens` …

Each series has 'R', 'P', and 'Q' branches. Each branch has several lines, where each line has several properties such as wavenumber and intensity.

`Cur_R_Peaks[14].wv` records the wavenumber of the line whose index in array Cur_R_Peaks is 14. Note that 14 here doesn't mean that the line is the **14th** line of this branch. The current top line's index of this R branch is in `Cur_R_Series.top`. Comparing with `Cur_R_Series.top`, we can know the real position of this line in the branch. This is like a double pointer in computer data structures. Fig 3.1 shows that when `Cur_R_Series.top` equals 9, `Cur_R_Peaks[14].wv` is the wavenumber of the sixth line in the R branch we have found up to this point during the searching process.

```
Index    J       wv          delta1       delta2      intens       comments
 9.          1019.771244   1.391835                 0.538795   Cur_R_Series.top
10.          1021.163079   1.374718   -0.017117   0.463053
11.          1022.537797   1.357109   -0.017609   0.391154
12.          1023.894906   1.339657   -0.017452   0.384100
13.          1025.234563   1.322407   -0.017250   0.388059
14.          1026.556970   1.304775   -0.017632   0.385666   Cur_R_Peaks[14]
15.          1027.861745   1.287316   -0.017459   0.383996
16.          1029.149061   1.269753   -0.017563   0.391489
17.          1030.418814   1.252379   -0.017374   0.412323   Cur_R_Series.bottom
18.          1031.671193   1.234256   -0.018123   0.292232
```

Figure 3.1: A sample used to explain Parm `Cur_R_Peaks[14].wv`.

For those parameters that have physical meanings, their values may be constants, or can be deduced during program running. Thus, there is an "askable" property for each parameter. If a parameter is askable, when its value is needed, the prompt is used and the value is taken from the user's answer.

Each parameter can also have its actual data type, such as integer, double, char, string, according to its factual data type, and a *stack* data type defined for MOSAA (for further details about the *stack* data type, see [13]).

3.3 Functions

Several processes in methanol spectroscopic assignment can be done using functions embedded in a rule.

Those functions can be classified into two groups: MOSAA functions and subroutines. There are no significant differences between these two types, just a trivial difference in the appearances in rules, as well as the fact that subroutines have more information hidden and all the required mathematical functions are included in MOSAA functions.

3.3.1 MOSAA functions

MOSAA functions can be classified into two groups:

normal MOSAA functions -

This kind of MOSAA function is almost identical to subroutines (see section 3.3.2) with the exception that it has a different appearance in the rule structure.

All mathematical functions belong to this type. For example:

```
== Cur_Series.branch, `R'
```

The MOSAA function `==` does an 'if equal' operation. The above example has the meaning : 'if the current assigning part is the R branch of the current assigning series'.

Other functions are used for special processing in running the inference engine, which also has some physical methanol spectroscopic assignment meaning in some sense. Function `FOUND`, for example, appears in the rule as:

```
FOUND  Sec_L_S_idx
```

where `Sec_L_S_idx` is a parameter introduced in section 3.2.

This function searchs for parameter `Sec_L_S_idx` in working memory and returns 'True' if this parameter is *found* in working memory. The physical meaning for this is: 'if the second line (of "Three Line Group") is already found'.

Each normal MOSAA function returns one value, which can be any legal data type defined. The values of some parameters may be modified inside a normal MOSAA function, this causes the problem of information hidden.

MOSAA-function rule functions -

These functions are not written as normal C++ functions; they are actual rules in the rule base. They are used (being called) as normal MOSAA functions.

To get one conclusion or to do one process, there might need to be several conditions existing. We could, certainly, encode this information into a normal MOSAA function or subroutine. This is not so good for maintenance as information is hidden too much.

As we mentioned in section 2.3, once we have three lines, we could do an expansion. This means that we can search for the next line in a certain wavenumber range and a certain intensity range. Sometimes, there are several candidates in this range. Thus we have several rules for selecting the most probable line from these candidates. Such a rule is shown below:

```
C_R200  IF   < (ABS Bias1), ERROR_TOLERANCE
           & > (ABS Bias2), ERROR_TOLERANCE
THEN
             Select  Pkf_idx1, Pkf_idx2, Bias1 , Bias2
           & Set ReturnI1, Pkf_idx1
           & Set ReturnI2, Pkf_idx2
           & Set Did_Select, 1
```

where `Select Pkf_idx1, Pkf_idx2, Bias1 , Bias2` selects one line (represented as Pkf_idx1 or Pkf_idx2, which is the peak finder file index of the line) according to its $\Delta 2$ bias with the previous line's $\Delta 2$. One must pay attention to the fact that, rules in MOSAA are order dependent. In this example, there are several rules before C_R200, which also deal with `Select`. Only when those previous rules have failed will this rule be tried.

Rule `C_R200` showing here is a MOSAA-function rule. It is a function in fact. `Select` is the function name and `Pkf_idx1, Pfk_idx2, Bias1, Bias2` are 4 arguments of this function. Function `Select` can be called in the same way as calling normal MOSAA functions. If a normal MOSAA function (written in C++) is written for `Select` instead of using MOSAA-function rule `C_R200`, the selection process information will be hidden.

Each MOSAA-function rule function can return more than one value, which can be any legal data type defined. These return values are put into parameters `ReturnI1, ReturnI2` ...as shown in rule `C_R200`. A MOSAA-function rule function also may modify some parameters, but these modifictions are visible to the user.

Section 3.7.2 also gives some discussion about how these MOSAA functions are used in the rule structure.

3.3.2 Subroutines

Subroutines are normal functions written in C++; they are one of the components of rules. Subroutines have very close resemblance to MOSAA functions when used in a rule.

Subroutines usually perform processing where information can be hidden. File access, user interface, and other modules which are difficult to code in rules are coded in subroutines.

Subroutine `show_sh` shows already assigned lines in the current series in spreadsheet style.

Subroutine `main_preprocess` does the main preprocess work of setting the working memory enviroment and the initial values of several parameters, to be ready for starting a spectroscopic assignment.

Subroutine `get_click_peak` returns the wavenumber of a line picked by the user in a graphical spectrum window.

Each subroutine returns one value, which can be any legal data type defined. The values of some parameters may be modified inside a subroutine, this causes same information hidden problem as normal MOSAA function.

3.4 Properties

Properties are associated with rules, and they give some additional control to the running of the inference engine, or make it easier to write or read some rules.

Here is a brief description of property **MATCH**. When a rule has a property such as:

```
MATCH L4, S_idx
```

then, besides the parameter `L4` being assigned the value `S_idx`, the other six `L` parameters-

```
L0, L1, L2, L3, L5, L6
```

are automatically assigned to

```
S_idx-4, S_idx-3, S_idx-2, S_idx-1, S_idx+1, S_idx+2
```

respectively. This makes writing current rules easier, and makes them more readable. Some other properties are very important in running the inference engine, and section 4.5 gives further details.

3.5 Explanation

The explanation part of a rule gives a brief English description of what this rule does. It explains the rule from the molecular assignment viewpoint, and is also used by the "Explanation Facility" during running of the inference engine.

3.6 Rules

The basic component of the MOSAA knowledge base is the rule base. Rules in MOSAA are written in plain ASCII characters and contained in file `_.rule` .

3.7 Rule structure

As mentioned in section 1.1, rules in the MOSAA KBS also have a normal **IF-THEN** structure with extra **Property** and **Explanation** parts. Fig 3.2 shows the MOSAA rule structure.

Fig 3.3 and Fig 3.4 are two sample rules from the rule base.

3.7.1 Rule categories

label in fig 3.2 contains the rule_id and the group this rule lies in. MOSAA rules are categorized into three groups: *G-Goal* , *C-Consequence* and *A-Antecedent* rules.

There are no major syntactical differences between these three types of rules, but in the inference engine, different kinds of rules act very differently. Section 4.2 gives a brief description about the role of each rule type in the inference engine.

rule_id shows the identification number of a rule; it can be any integer number which is in "int" range.

label **IF** $condition_1$
$condition_2$
... Premise
$condition_n$

THEN $conclu_1$
$conclu_2$
... Conclusion
$conclu_n$

$prop_1$
$prop_2$
... Property
$prop_n$

/* .... Explanation

*/

Figure 3.2: Rule structure.

3.7.2 Conditions

condition in the Premise can be one of the following clauses:

single parameter -

If the parameter's value is known and $\neq 0$, this condition becomes true.

MOSAA function -

If this MOSAA function returns a value $\neq 0$, this condition becomes true.

condition_1 in fig 3.3 calls a MOSAA function condition. < is the name of the function, and the following two symbols **`Cur_R_Series.top`** and **`Cur_R_Series.top_of_three`** are two arguments of this function. The argument can be a single parameter, an expression, or even a bracketed MOSAA function or subroutine.

```
C_R38  IF   <  Cur_R_Series.top,Cur_R_Series.top_of_three
                                                 /%condition_1%/
         &  FOR i= Cur_R_Series.top_of_three-1;
                     Cur_R_Series.bottom_of_three /%condition_2%/
              {
                 Transfer_Line_R_To_P  i         /%loop_clause_1%/
               & Transfer_Line_R_To_Q i          /%loop_clause_2%/
               & UNFOUND R_To_Q_Pro_L            /%loop_clause_3%/
              }
         &  FOR i=Cur_R_Series.top_of_three;
                     Cur_R_Series.bottom_of_three  /%condition_3%/
              {
                 RPQ_Confirm i
              }
       THEN
            =  Transfer_TJ_To_P, 1                         /%conclu_1%/
       /*
           IF    there are already four R branch  lines which includes
                 three_lines and one line above the top of the
                 three_lines
             AND
                 from these four R branch lines, can find corresponding
                 P and Q lines
             AND
                 using these R, P,Q branch lines, we have confirmed
                 three_lines
           THEN
                 Transfer three_lines to  P has been done
       */
```

Figure 3.3: A sample consequence rule.

```
C_R250 IF   UNFOUND Stop_Transfer
         &  UNFOUND Cur_Series.K
         &  == Search_Dire, 'P'
         &  Set Pkf_idx1, ( $$get_P_from_R(Cur_R_Peaks[S_idx].wv,
                Cur_R_Peaks[S_idx].J))  /%condition_4%/
         &  Pkf_idx1
       THEN
            Set TEMPI1, S_idx+2
         &  Set Cur_P_Peaks[TEMPI1].pkf_idx, Pkf_idx1
         &  Set Cur_P_Peaks[TEMPI1].J, Cur_R_Peaks[S_idx].J+2
         &  = Cur_Found_P_Line, TEMPI1
         &  Transfer_Line_R_To_P  S_idx
       /* IF    Transfer has not been stopped
            AND Current series' K value is already known
            AND Searching from R branch to P branch
            AND calling subroutine 'get_P_from_R' has found the
                corresponding P branch peak for R branch peak S_idx
          THEN
                this MOSAA-func rule is true (Transfer_Line_R_To_P S_idx).
            AND
                record corresponding information for this current found
                P branch peak.  Since Cur_Found_Line_P_Line value is
                determined by '=' instead of 'Set', it may invoke antecedent
                rules to do further processing
       */
```

Figure 3.4: A sample MOSAA-function rule.

Table 3.1: The three types of loops.

loop	condition value
FOR	During the loop, anytime the loop body fails the condition fails
ANYIF	During the loop, anytime the loop body succeeds the condition becomes true
DO	Just execute the clauses in the loop body; the condition is always set to be true

loop_clause_1 calls a special kind of MOSAA function, which in fact is a *MOSAA-function rule* function. This kind of MOSAA function is not a C++ function; instead it is a consequence rule and can only be a consequence rule.

Fig 3.4 shows this *MOSAA-function rule.* Conclusion condition `Transfer_Line_R_To_P S_idx` shows this is a *MOSAA-function rule.* We can see that for the caller, *loop_clause_1* in CR_38 *condition_2*, there is no difference in calling a *normal* MOSAA function, or a *MOSAA-function rule* function.

subroutine -

If this subroutine returns a value $\neq 0$, this condition becomes true.

A subroutine condition is similar to a normal MOSAA function condition, with a trival difference in format.

loop -

Loop is a special type of condition. Each loop has a head part and a body part. The head part shows the loop type and sets the start value, end value and step value of the loop variables. The body part is a group of clauses, which can be one of the three previously introduced conditions. When all the clauses in the loop body are true, this loop body becomes true.

There are three kinds of loops, and Table 3.1 gives a brief description of them.

An example showing the `FOR` loop is given previously in Figure 3.3. There are three loop clauses inside the first `FOR` loop body. Only when these three loop clauses are always true stepping through the whole loop, this loop returns true. In any step, as long as one clause fails, this `FOR` loop returns false.

If we change this loop from `FOR` to `ANYOF`, as long as these three clauses inside the loop body all become true in one step, this loop returns true.

`DO` loop always returns true.

3.7.3 Conditions of conclusion part

$concl u_i$ in Conclusion can be one of the following clauses:

MOSAA function -

If the MOSAA function is a normal one, simply call it to do the corresponding process. If it is a *MOSAA-function rule* function name, which means the current rule itself is a *MOSAA-function rule* being called, then do nothing.

For example, rule `C_R250` in Fig 3.4 is a *MOSAA-function rule*. Conclusion condition

`Transfer_Line_R_To_P S_idx` shows this is a *MOSAA-function rule*. This rule is tried when the MOSAA function name appears in some other rules, such as in `C_R38`. When this rule is fired, it is as if the MOSAA function is called. Therefore, all the other conditions in the conclusion are done, except the *MOSAA-function rule* function condition.

subroutine -

Call this subroutine.

loop -

Do this loop (can only be **FOR** or **DO**).

All the parameters appearing in the conclusion must already be known; otherwise an error message is provided.

Chapter 4

Inference Engine

The MOSAA system inference engine combines *backward chaining* and *forward chaining*, as well as two special mechanisms *TRY* and *restart*. Appendix C of the *MOSAA Developer's Guide* gives diagrams of this inference engine [13].

4.1 Working memory

Working memory (WM) in knowledge-based systems can also be called the *fact base* which stores current facts in a certain way.

WM in MOSAA stores current values of parameters. The inference engine puts the value of a parameter into WM when the value of this parameter is determined or modified; it searches for the value of a parameter from WM whenever pit needs the value of this parameter.

Due to the special mechanisms *TRY* and *restart* (discussed later in section 4.5), certain states of WM must be stored for future usage. WM store is used to save the working memory in difference states while running the inference engine.

4.2 Three types of rules

As we mentioned, there are three groups of rules in the inference engine, and each group has a different role.

1. **Goal Rule**

   The goal rule starts the inference engine by trying to determine if the premise in the goal rule is true.

   Fig 4.1 is a goal rule which starts the whole assignment engine. At first it does several initial processes. If these finish successfully, it then tries to determine if parameter `All_Assign_Done` is true, which starts the whole engine.

```
G_R1     IF     $main_preprocess()
           &    All_Assign_Done
         THEN
                $final_step()
```

Figure 4.1: A sample goal rule.

2. **Consequence Rules**

   Consequence rules are used in the backward chaining. When the inference engine needs to determine a parameter's value, the consequence rules are tried one by one. The consequence rule is tried only when it has a MOSAA function or subroutine condition, which can determine the inquiring parameter's value (modify type of this parameter must be 'r').

   Rule `C_R38` in Fig 3.3 is a consequence rule. When the parameter `Transfer_TJ_to_P` value needs to be determined, `C_R38` is tried, since there is a MOSAA function '`=`' in the conclusion which can determine the value of parameter `Transfer_TJ_to_P`.

If the current fired consequence rule determines or modifies a parameter (the modify type of this parameter in its MOSAA function or subroutine must be 'r' or 'm'), forward chaining is invoked.

3. **Antecedent Rules**

   Antecedent rules are used in forward chaining. Once a parameter's value is determined or modified during or after doing the conclusions of one rule (which can be a Consequence or Antecedent rule), the forward chaining is invoked. An antecedent rule is tried when its premise has the parameter whose value has just been determined.

   As long as one antecedent rule is fired, no more antecedent rules are going to be tried, unless being forced by the *Relative* property.

   When there are any unknown parameters in the premise, this rule is skipped, unless it has the *INVOKE* property.

   As for a consequence rule, when the current fired antecedent rule determines or modifies a parameter, more forward chaining is invoked. Otherwise, the inference engine returns to backward chaining.

   Fig 4.2 shows an antecedent rule. During the inference engine running, once the value of parameter `Fir_L_S_idx` is determined, several antecedent rules are tried. `A_R3` is one of those antecedent rules to be tried. If both of the conditions in the premise are true, this rule is fired, and the corresponding conclusions are done.

4.3 History tree

The history tree in MOSAA records the main path of the inference engine deduction. In the MOSAA inference engine, the history tree is used not only for the explanation

```
A_R3    IF     Fir_L_S_idx
           &   UNFOUND ROUGH_2B
        THEN
               Set TEMPI1 , Cur_Peaks[Fir_L_S_idx].pkf_idx
          &    Set Cur_Peaks[Fir_L_S_idx].wv , PKF[TEMPI1].wv
          &    Set Cur_Peaks[Fir_L_S_idx].intens, PKF[TEMPI1].intens
          &    Set Cur_Peaks[Fir_L_S_idx].series_no, Cur_Series_No
          &    Set Cur_Peaks[Fir_L_S_idx].zone_no,
                                    ($get_zone_no(TEMPI1) )
          &    $show_peak(TEMPI1)
       /*IF     Find the first line
         THEN
                set the corresponding value to the parms
       */
```

Figure 4.2: An antecedent rule: A_R60.

facility, it is also very important for one special mechanism called *TRY*, which is discussed in section 4.5.

From each goal rule, the inference engine starts building a history tree. There are two kinds of nodes in the tree; a consequence history tree node and an antecedent history tree node. An example architecture of a history tree is shown in Fig 4.3.

As shown in the figure, each node has a unique *pos* number. The *pos* number increases as the deduction process proceeds. Main nodes in the tree are consequence history tree nodes, where each node can have several antecedent history tree nodes associated with it. Due to the inference engine complexity, where forward chaining also could invoke backward chaining as mentioned in section 4.2, the building of history tree nodes stops at antecedent history nodes. This means that even though an antecedent rule could invoke a consequence rule, it won't build consequence history tree nodes as branches under it. This will cause some loss of information, but this situation only happens when the `INVOKE` property is used (refer to section 4.5), which is seldom used.

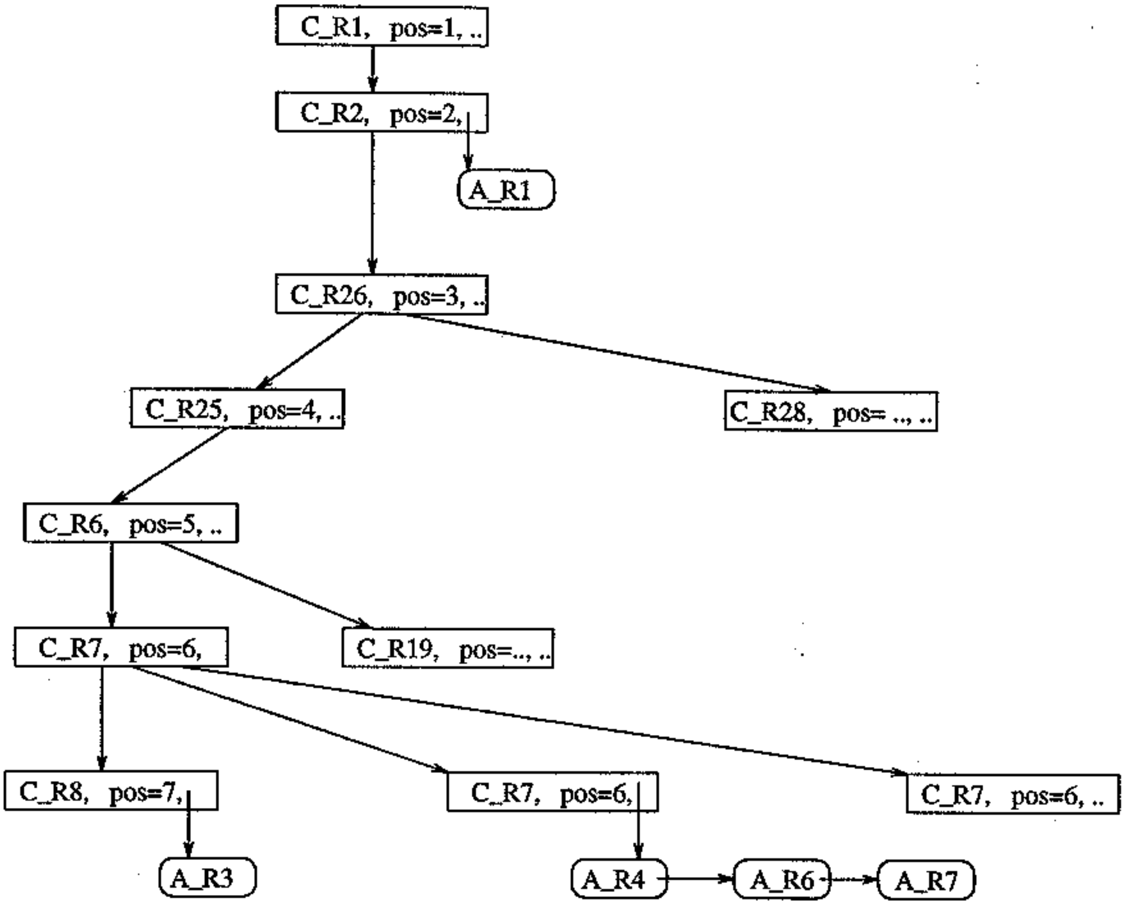


Figure 4.3: Example architecture of a history tree.

4.4 *monitor*, *findout* and 'WM store'.

MOSAA uses the backward chaining algorithms of *monitor* and *findout.*

The goal rule starts the whole inference engine by invoking the *monitor* algorithm. The *monitor* algorithm tries to judge if conditions in the premise of the goal rule are right or not. In order to do that, all the parameters in the goal rule must be known, which initially is impossible, and thus algorithm *findout* is invoked.

findout looks up the whole consequence rule base; when the conclusion of a consequence rule has a function (MOSAA function or subroutine) which can deduce the value of the parameter searched, this rule is tried as we mentioned in section 4.2.

To try a consequence rule means that a lower layer mechanism *monitor* is invoked for determining if this rule can be fired or not. *monitor* may invoke *findout* again in order to get the value of parameters needed.

As mentioned in section 4.1, for later *restart* and *TRY* purposes, WM as well as its corresponding position number in each stage is stored in WM store. This process, recording WM in corresponding positions, is done whenever *monitor* is invoked to judge if one rule is true or not. If this rule fails, before getting out of the current monitor, the corresponding position's WM is deleted from WM store. When this rule is successfully fired and all the conclusions have been made, the corresponding position's WM is also removed from WM store. Fig 4.4 shows the situation changing in WM store during a simple deduction process.

4.5 Special properties

Besides the basic backward chaining and forwarding chaining, some special properties of rules also control the inference engine running.

4.5.1 MATCH

MOSAA is used for assisting in the assignment of spectroscopic lines. Quite a few rules in the knowledge base deal with the relationships among several neighboring lines. To make writing rules easier, and make them more readable, property `MATCH` is used.

When a rule has a property such as

```
MATCH L4, S_idx
```

then, besides the parameter `L4` being assigned the value `S_idx`, the other six `L` parameters

```
L0, L1, L2, L3, L5, L6
```

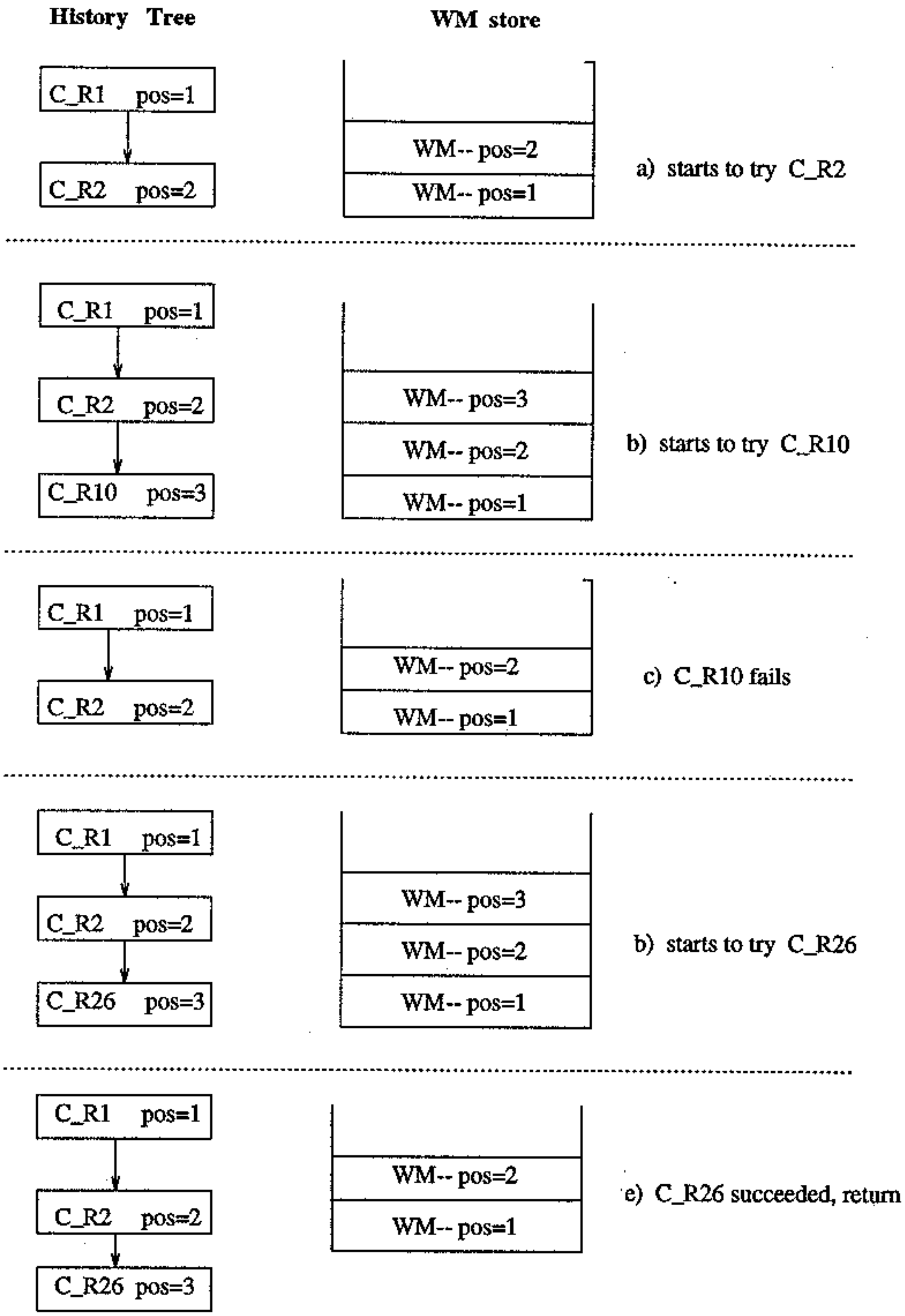


Figure 4.4: WM store during deduction.

are automatically assigned to

`S_idx-4, S_idx-3, S_idx-2, S_idx-1, S_idx+1, S_idx+2`

respectively.

4.5.2 INVOKE

This property can only appear in an antecedent rule. Normally the rule is skipped, if it has an unknown parameter. If the rule has this `INVOKE` property, 'simple' backward chaining is invoked to try to determine the value of this unknown parameter. The reason that we call it 'simple' backward chaining is that no forward chaining is invoked during this 'simple' backward chaining.

4.5.3 Relative

This property can only appear in an antecedent rule. It can be

Relative 'A', *rule_id* //first case

or

Relative 'C', *rule_id* //second case

When a rule with such a property is fired and all the conclusions are done, in the first case, the corresponding antecedent rule with that *rule_id* is invoked. For example, Fig 4.5 shows a group of A_R rules.

This group of antecedent rules are used to do the processing after the second line of the "Three Line Group" has been found. If A_R4 is fired, A_R6 and A_R7 are successively tried.

The second case invokes a special mechanism *restart*. Once the consequence rule with *rule_id* is the ancestor of the consequence rule which invokes the current antecedent rule, the inference engine will restart from that particular point. The complete

```
A_R4    IF    Sec_L_S_idx
        THEN
              Set TEMPI1, Cur_Peaks[Sec_L_S_idx].pkf_idx
          &   Set Cur_Peaks[Sec_L_S_idx].wv, PKF[TEMPI1].wv
          &   Set Cur_Peaks[Sec_L_S_idx].intens, PKF[TEMPI1].intens
          &   Set Cur_Peaks[Sec_L_S_idx].series_no, Cur_Series_No
          &   show_peak(TEMPI1)
          &   Set Top_L_S_idx, (Minimum Fir_L_S_idx, Sec_L_S_idx)
          &   Set Bottom_L_S_idx, (Maximum Fir_L_S_idx,Sec_L_S_idx)
        #  Relative 'A', 6
         & Relative 'A', 7

A_R6   IF   Sec_L_S_idx
         &  > Cur_Peaks[Bottom_L_S_idx].wv, 0
         &  > Cur_Peaks[Top_L_S_idx].wv, 0
       THEN
            Set Cur_Peaks[Top_L_S_idx].delta1,
                   Cur_Peaks[Bottom_L_S_idx].wv-Cur_Peaks[Top_L_S_idx].wv

A_R7   IF   Sec_L_S_idx
       THEN
            REMOVE  Search_Zone_No
         &  REMOVE  S_Low_Range
         &  REMOVE  S_High_Range
         &  REMOVE  I_Low_Range
         &  REMOVE  I_High_Range
```

Figure 4.5: A sample of using property `Relative 'A', x`.

environment (the value of all parameters) are reset at that point, except for some parameters whose values are reserved by the MOSAA function `RESERVE`. Fig 4.6 shows an example.

```
C_R13   IF   FOUND Sec_L_S_idx
          &  UNFOUND Thi_L_S_idx
          &   .........
        THEN
                =  Thi_L_S_idx,  TEMPI1

C_R18  IF   Thi_L_S_idx
       THEN
              =  Thi_L_Found, 1


C_R105  IF   UNFOUND  Thi_L_S_idx
       THEN
                =  Thi_L_S_idx, 0

A_R32  IF   !Thi_L_S_idx
         &  Set TEMPI1, ( Pop_Line Line_Reserve_Stack, Sec_L_S_idx )
         &  TEMPI1
       THEN
            Set Cur_Peaks[Sec_L_S_idx].pkf_idx, TEMPI1
         &  = Sec_L_S_idx, Sec_L_S_idx       /%just for invoking purposes%/
         &  RESERVE Cur_Peaks[Sec_L_S_idx].pkf_idx
         &  RESERVE Cur_Peaks[Sec_L_S_idx].zone_no
         &  RESERVE Sec_L_S_idx, 'y'
         &  RESERVE Line_Reserve_Stack
       #Relative 'C', 18
```

Figure 4.6: An example of using property ``Relative `C´,x``.

Basically, `C_R18` tries to find the third line of the "Three Line Group". If `C_R13` fails, parm `Thi_L_S_idx` is not determined; then the premise of `C_R105` becomes true and `C_R105` is fired, thus invoking antecedent rules. If `A_R32` is fired, which means that there are some other second lines that can be used, after some processing, the inference engine restarts the deduction from the consequence rule `C_R18`. All the modifications of the parameters which were done up to this point are removed, and since we want to keep the information that another second line has been chosen, 'RESERVE' is used to save the new second line information. The history tree in Fig 4.7 illustrates this process.

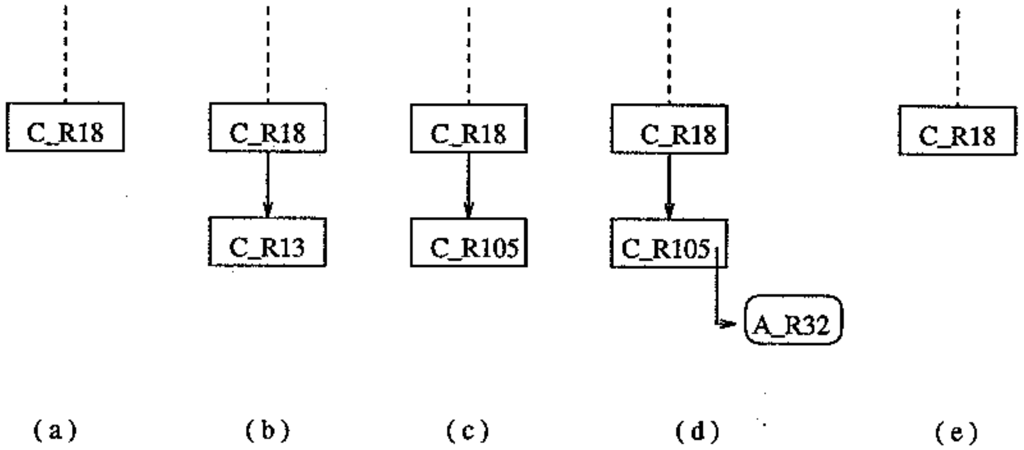
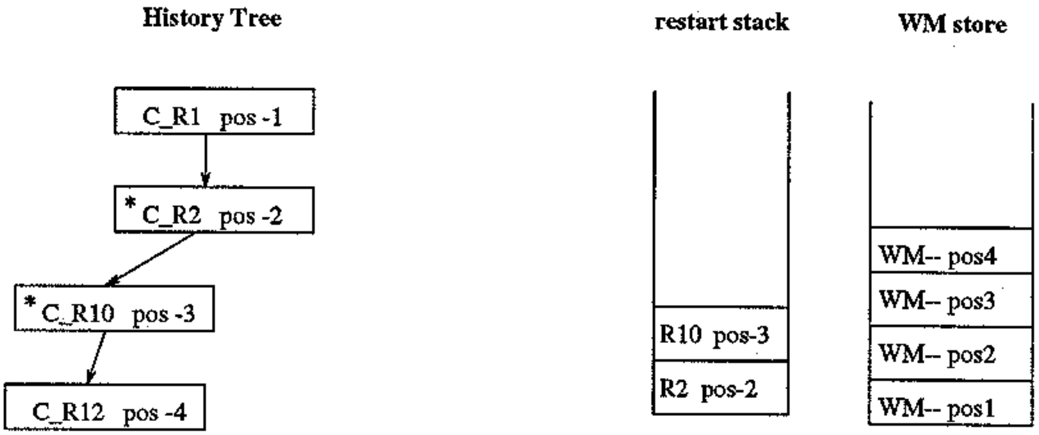


Figure 4.7: History tree illustrating the process of using rules in Fig 4.6.

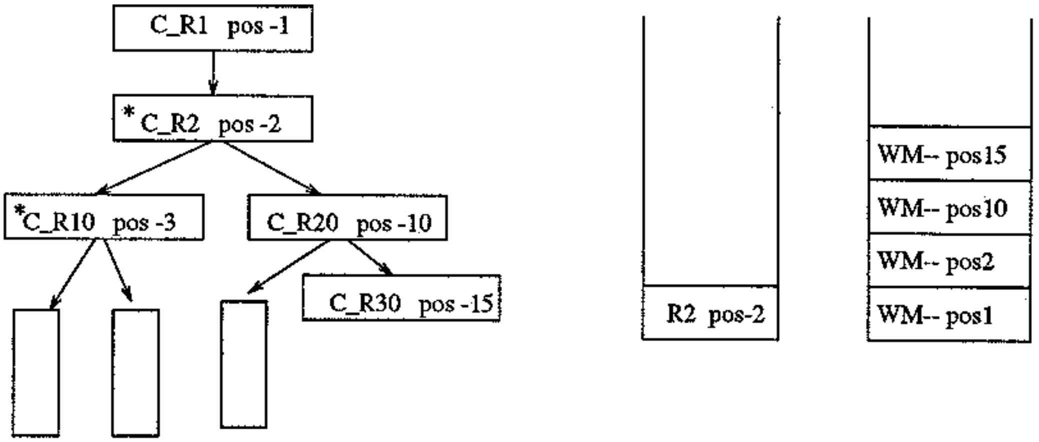
To implement this '*restart*', WM store and a restart_stack are used.

During the deduction, before trying a candidate consequence rule, properties of this rule are considered. When this rule is a relative rule of some antecedent rules, it has an 'ISRELATIVE' property assigned in the MOSAA preprocess as will be mentioned in section 5.2. Therefore, the position number with the rule id of this rule is pushed onto the restart_stack. If later this rule is successfully fired and all the conclusions have been done, and it is ready to return back to the higher rule which invoked it, this rule is removed from the restart_stack. If the rule fails, it is removed from restart_stack as well.

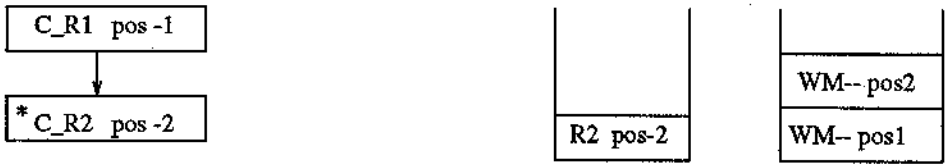
Fig 4.8 shows relative situations for explaining the restart process. In Fig 4.8 b), assume that `C_R30` determines a parameter and invokes an antecedent rule. This antecedent rule has a relative rule which is `C_R2`. The MOSAA inference engine looks up in the restart stack and finds rule2 with its position number. Therefore the restart position is 2 and the inference returns to that point; the current WM is reset by WM



a) starts to try rule C_R12



b) C_R10 branch successfully fired, starts try C_R30



c) after restart rule C_R2

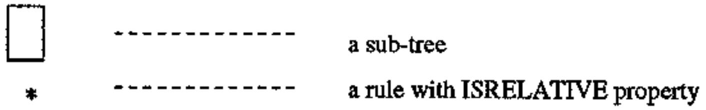


Figure 4.8: The restart process.

with position number 2 from WM store, and the deduction restarts from this point.

Now assume in Fig 4.8 b), the antecedent rule invoked by `C_R30` has a relative rule `C_R10`. Since there is no rule 10 in the restart stack, which means rule `C_R10` is not the ancestor of rule `C_R30`, restart can't be invoked. MOSAA will give an error message if this situation occurs. The rule base must be written so as to avoid this situation.

4.5.4 TRY

This property can only appear in a consequence rule. The basic idea is that, once a consequence rule is fired, the conclusion may have more than two choices. If, later on, the inference engine gets stuck, it can come back to make another choice.

`C_R9` is a rule with the "TRY" property, which determines the search range for the second line of the "Three Line Group" (see Fig 4.9). Once `C_R10` (which invoked `C_R9`) fails, the environment is reset, and the inference engine can come back to pick another choice of the search range.

To implement this `TRY` property, the WM store, History tree and TRY store are used.

Except for the basic information stored in the history tree as mentioned in 4.3, special tags are used in consequence history tree nodes for property `TRY` purposes. When a consequence rule is successfully fired, if it has the `TRY` property, tag **T** is assigned to the corresponding consequence history node. In the mean time, all consequence nodes in the path from this node to the root are assigned the tag **G**.

A TRY store is used to store TRY information. Each item in the TRY store has the structure as shown in Fig 4.10.

When only one rule such as `C_R9` has the `TRY` property, the implementation is simple. If there are several rules having the `TRY` property, they may be in the same history tree, and we need to decide the consequence of the rules to be tried.

To explain the implementation of property `TRY`, a group of sample rules in Fig 4.11 are used. These rules are not the real rules in the rule base, since real rules are too

```
C_R9    IF   FOUND Fir_L_S_idx
          &  UNFOUND Sec_L_S_idx
          &  == Cur_Series.branch, 'R'
        THEN
             =  Search_Zone_No,  Cur_Peaks[Fir_L_S_idx].zone_no+1
          &  Set TEMPI1,  Search_Zone_No-1
          &  Set TEMPD1, Cur_Peaks[Fir_L_S_idx].wv
                                + Zone_Area[TEMPI1].av_sp
          &  =  S_Low_Range,  TEMPD1 - S_RANGE1
          &  =  S_High_Range, TEMPD1 + S_RANGE1
          &  =  I_Low_Range, Cur_Peaks[Fir_L_S_idx].intens - I_EXT
          &  =  I_High_Range, Cur_Peaks[Fir_L_S_idx].intens+I_EXT
        #TRY
         {
             =  Search_Zone_No, Cur_Peaks[Fir_L_S_idx].zone_no-1
          &  Set TEMPD1, Cur_Peaks[Fir_L_S_idx].wv
                                      - Zone_Area[Search_Zone_No].av_sp
          &  =  S_Low_Range, TEMPD1 -  S_RANGE1
          &  =  S_High_Range, TEMPD1 + S_RANGE1
          &  =  I_Low_Range, Cur_Peaks[Fir_L_S_idx].intens - I_EXT
          &  =  I_High_Range, Cur_Peaks[Fir_L_S_idx].intens + I_EXT
         }
        /*_ P39 R38,39
          IF     first line of three lines is found(!=0)
          THEN   search the second line in the zone preceding the current
                 zone (zone which first line lies in),the wv search range
                 for this is  the first line - the distance between two
                 zones +-S_RANGE1 ( which is the search extension)
                 the intens of the second line must be in range intens of
                 the first line  +-I_EXT
          Property
              also can try:
                 search the second line in the zone following current zone
                 (zone which first line lies in),the wv search range for
                 this is  the first line - the distance between two zones
                 +-S_RANGE1 ( which is the search extension)
                 the intens of the second line must be in range intens of
                 the first line  +-I_EXT
*/
```

Figure 4.9: A sample rule using the TRY property.

pos	rule	try_num	trys	pre_try

rule -- points to the corresponding consequence rule
try_num -- the number of TRY properties in this rule
trys -- an array containing points which point to TRY conclusion
clauses in this rule
pre_try -- the previously tried conclusion clause

Figure 4.10: The structure of an item in the TRY store.

long and complicated to be demonstrated here.

Fig 4.12 a) is the history tree. During the deduction, when rule `C_R4` is fired, its conclusions are done. Since this rule has the `TRY` property, the corresponding information is pushed onto the TRY Store, which is the bottom item in Fig 4.12 b). The `try` link contains `TRY #1`. `pre_try` points to the original conclusion part (`#orig`) since no TRY has yet been carried out.

Rules `C_R6` and `C_R2` succeed one after another. This results in the TRY Store as shown in Fig 4.12 b).

Whenever a rule *x* which has the TRY property is successfully fired, tag 'Tx' is added to the corresponding node in the history tree. All the antecedents of this node in the history tree have a 'Gx' tag added. The tag is always added to the head of the existing tag list. As shown in Fig 4.12 a), node pos-2 in the history tree has tag G2-G6-G4, due to successfully firing rules `C_R4`, `C_R6` and then `C_R2`. Node pos-4 has a tag 'T4' since rule `C_R4` has the TRY property.

Suppose now the inference engine is trying branch B2, which is condition `func(X,Y,Z)`. At this point, the try store is as shown in Fig 4.12 b), where node `#orig` is the original conclusion, and `#1` is the first try clause as shown in the rules (Fig 4.11). Now `X, Y, Z` have values as the first row (Orig try) in Table 4.1. If `func(X,Y,Z)` is '$Y > Z > X$', condition B2 is satisfied and rule `C_R1` is fired. If `func(X,Y,Z)` is something else such

```
C_R1  IF  !=  A, 0
        & func(X,Y,Z)
      THEN
          conclusion


C_R2  IF  >  B, 3
        & != D, 0
      THEN
          = A, 1
        & = X, 3  /%#orig%/
      # TRY
        {   = A, 1
          & = X, 4
        }         /% #1 %/
      & TRY
        {   = A, 1
          & = X, 5
        }         /% #2 %/


C_R3  IF  == C, 1
      THEN
          = B, 4
```

```
C_R4  IF    == user_input, 'Y'
      THEN
            = C, 1
        &   = Z, 4  /%#orig%/
      # TRY
        {   = C, 1
          & = Z, 3
        }           /% #1 %/

C_R5  IF   >  Y, 0
       THEN
            = D, 100


C_R6  IF    == user_input, 'IR'
      THEN
            =  Y, 6 /%#orig%/
      # TRY
        {  =  Y, 5
        }           /%#1%/
       & TRY
        {  =  Y, 4
        }           /%#2%/
```

Figure 4.11: A group of hypothetical rules used to illustrate the try process.

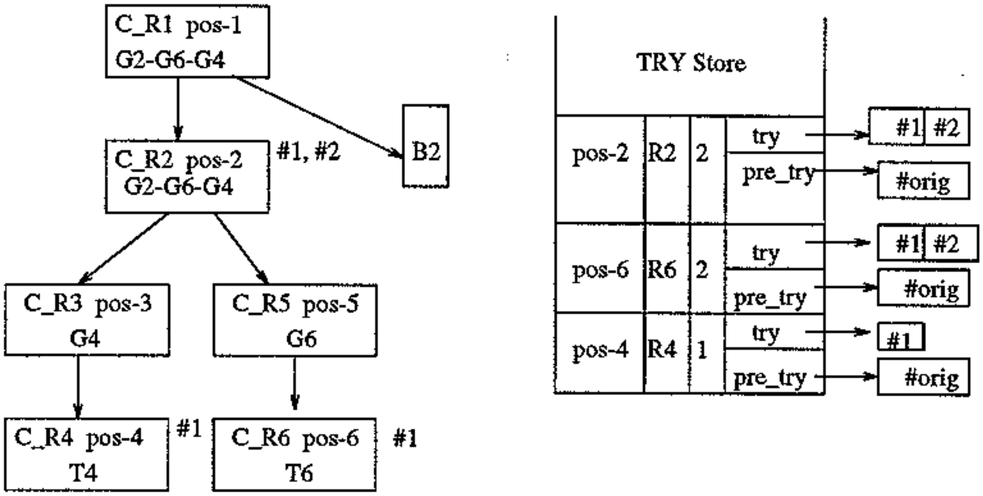
as 'X=Y=Z', condition B2 is not satisfied and rule C_R1 **is going to** fail.

Before we give up on this rule, we look up in the history tree to see if any of its descendants can be tried. As seen in Fig 4.12 a), node C_R1 has tag G2-G6-G4, which means there are several other choices to try. G2 is used first, thus the rule in pos-2 (i.e. C_R2) is going to be tried and flag **TRY** is set here[1].

Before *TRY* starts, the whole inference engine restarts from this point (pos-1).

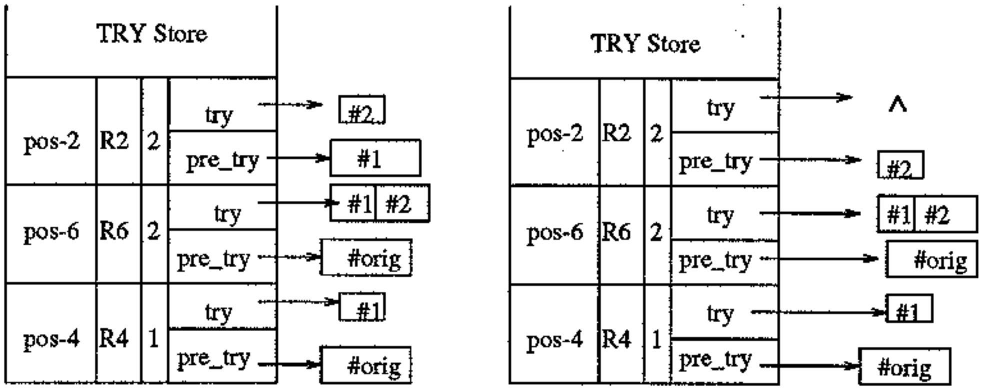
---

[1] When the **TRY** flag is on, one rule ahead is going to be tried (in this case, rule C_R2 is the rule to be tried). The **TRY** flag will be switched off when deduction gets to TRY rule C_R2 and has finished doing **TRY** conclusion.



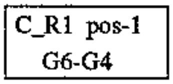
a) History tree after C_R2 succeeds.

b) initial try store (no try has been done)

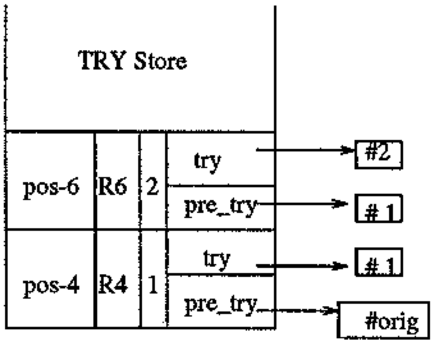


c) try store after using #1 as C_R2's conclusion.

d) try store after using #2 as C_R2's conclusion

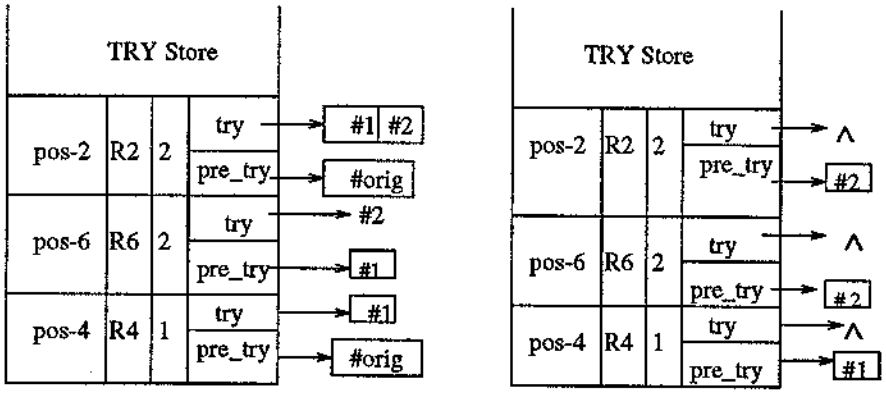


e) history tree after C_R2 fails, due to the fact that no try is available for C_R2 in the TRY store



f) try store when try #1 of rule CR_6 is used as conclusion

Figure 4.12: TRY process.



g) #2 of C_R6 is used as the conclusion for C_R6 now, and since C_R2 succeeds, its try cases are stored in the TRY store.

h) #1 of C_R4 is used as the conclusion for C_R4 while #2 of C_R6 is used as the conclusion for C_R6. #2 is used as the conclusion as C_R2. If branch B fails still, no try can be used any more.

Fig 4.12 (continued)

This process is similar to the *restart* mechanism. WM is reset, and the corresponding environment including the history tree is reset.

The deduction restarts from C_R1 (pos-1). The premise of Rule `C_R4` is true. Although now TRY is on (**TRY** flag is on) and rule `C_R4` has the **TRY** property, since `C_R4` is not the rule to be tried this time (rule `C_R2` is the rule to be tried as defined previously), the conclusion part pointed to by `pre_try` in the TRY Store (which is `#orig` for rule `C_R4`) is used. Therefore, Z is set to be 4 as before. The same process is done in Rule `C_R6` (pos-6) and Y is set to be 6 as before.

The deduction in the history tree comes back to `C_R2` (pos-2). Two conditions of the premise of `C_R2` are true (due to the same deduction path followed so far). `C_R2` is the rule to be tried, the conclusion now to do is `#1` according to the TRY Store instead of `#orig`, and the TRY Store becomes as shown in Fig 4.12 c). X becomes 4 and flag **TRY** then is switched off.

At this point, X, Y, Z are as shown in the second row (1st try) in Table 4.1. If

Table 4.1: Values of X,Y,Z in each try.

Try	X	Y	Z
Orig	3	6	4
1st	4	6	4
2nd	5	6	4
3rd	3	5	4
4th	4	5	4
5th	5	5	4
6th	3	4	4
7th	4	4	4
8th	5	4	4
9th	3	6	3
10th	4	6	3
11th	5	6	3
12th	3	5	3
13th	4	5	3
14th	5	5	3
15th	6	5	3
16th	3	4	3
17th	4	4	3
18th	3	4	5

`func(X,Y,Z)` is something like '$X = Z$ AND $Y > X$', rule `C_R1` is fired. Otherwise, another TRY is invoked and Fig 4.12 d) shows the results in the TRY Store after try `#2` of `C_R2`.

When branch `B2` (function func(X,Y,Z)) still fails, TRY is invoked once more. When it gets back to pos-2, no more TRYs can be obtained from the TRY Store. Therefore rule `C_R2` fails and no relative tags (`T2, G2`) are set in the history tree. The sub-tree from pos-2 is cut from the history tree due to the failure of `C_R2`.

The history tree now is as shown in Fig 4.12 e). The head of the tag list for node pos-1 now is G6, and according to this, pos-6(`C_R6`) is going to be tried. TRY starts and gets `C_R6` (pos-6). Since this is the rule to be tried, TRY `#1` of rule `C_R6` is used as the conclusion instead of the original conclusion `#orig`, which sets Y to be 5. The TRY Store then is as shown in Fig 4.12 f), and, since TRY succeeds, TRY then is switched off.

The deduction then gets back to rule `C_R2` (pos-2). Now flag **TRY** has been switched off, and the process for `C_R2` is the normal case. Therefore, the TRY information of `C_R2` is pushed into the TRY Store as shown in Fig 4.12 g) and the history tree becomes the same as in Fig 4.12 a). 'X, Y, Z' now have the values shown in the '3rd try' row of Table 4.1.

If `func(X,Y,Z)` is '$X > Y > Z$', this means all the combinations of 'X, Y, Z' in Table 4.1 before the last row won't satisfy it. Then branch `B2` fails all the time, and `C_R1` finally gets to the last TRY. The TRY Store is as shown in Fig 4.12 h). Now 'X, Y, Z' have the values shown in the 18th try in Table 4.1, and it satisfies '$X > Y > Z$'; thus rule `C_R1` is fired.

If `func(X,Y,Z)` is '$Z > Y > X$', which can't find any satisfactory combinations of 'X, Y, Z' in Table 4.1, rule `C_R1` finally will fail when all the `TRY`s in the `TRY` store have been used up.

As long as one of the TRY cases makes `B2` true, `C_R1` becomes true.

4.5.5 Mixing `TRY` and `Relative`

One must be very careful when mixing the `TRY` and `Relative` (restart) properties, since after restart, the deduction path may be changed by the parameters which are reserved, which can make 'TRY' fail. We will use an example to briefly discuss this problem; Fig 4.13 gives a group of hypothetical rules used to illustrate this.

Assume that the inference engine wants to determine the value of parameter `Final_Parm`. Up to this point, we say the environment is *environment*1. The deduction path at first is as shown in Fig 4.14 (a). Rule `C_R3` is fired, and `C_R4` is tried to determine the second condition of `C_R2`. `C_R4` fails since `Parm_A` is less than 10. Then `C_R5` is fired, parameter `Parm_B` is determined to be 0 and this invokes `A_R1`. `A_R1` is true and the property: `#Relative `C´, 2` restarts the deduction from `C_R2`. This time, `Parm_A` is already known (is set to be 12 by `A_R1`) since it was reserved by `A_R1`,

```
C_R1    IF     Parm_C
          &    == Parm_C, 2
        THEN
               = Final_Parm, 1

C_R2    IF     Parm_A
          &    Parm_B
        THEN
               =  Parm_C,  1
        # TRY { = Parm_C, 2}

C_R3    IF     function_1
        THEN
               =  Parm_A, 2

C_R4    IF     >  Parm_A, 10
        THEN
               =  Parm_B, 4

C_R5    IF     UNFOUND  Parm_B
        THEN
               =  Parm_B,0

C_R6    IF     UNFOUND  Final_Parm
        THEN
               = Final_Parm, 0
```

```
A_R1  IF  !parm_B
      THEN
          = Parm_A, 12
        & RESERVE  Parm_A
      #Relative 'C', 2
```

Figure 4.13: A group of hypothetical rules used to illustrate the problem of mixing the use of 'Relative' and 'TRY'.

and the deduction path changes to look like Fig 4.14 (b). Now, `C_R4` succeeds and determines `Parm_B`, which makes the left-hand-side of `C_R2` become true, and `Parm_C` is set to 1.

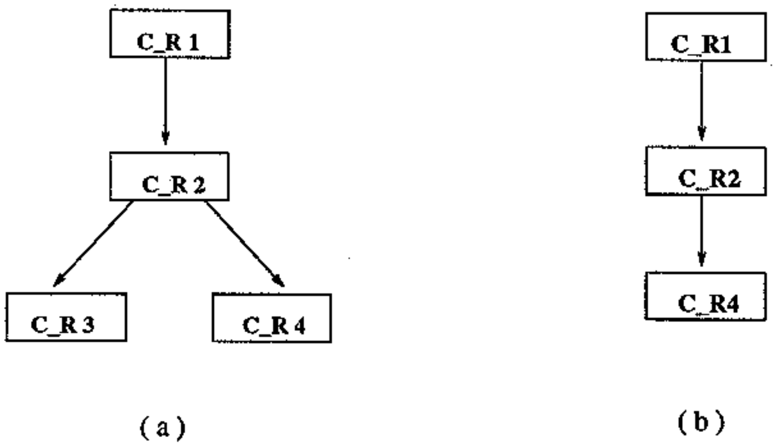


Figure 4.14: Simple deduction paths for the rules of Fig 4.13.

Returning to `C_R1`, condition 2 fails, before `C_R1` fails, and the engine starts to search for "TRY" in `C_R1`'s branches, and finds one in `C_R2`. The environment is reset as at the very beginning (*environment1*), and the engine starts deduction from `C_R1` again. The deduction path now becomes Fig 4.14 (a) again, while it should be the same as Fig 4.14 (b). Since the deduction path changes, "TRY" fails.

This case which mixes the `TRY` and `Relative` properties should be avoided when adding or modifying rules in the rule base. When a TRY rule is the Relative rule of an antecedent rule, one should be very careful.

Chapter 5

Implementation

The MOSAA system was developed on the Linux(Unix) environment, which includes the following components:

GNU C++ compiler (*g*++)
lex
bison
X Window System/XView

This software runs on a Linux workstation, with a Pentium 100MHz processor, 16MB RAM, and 1.2GB hard disk.

There are two versions of MOSAA; the *command line* version and the *xview* version. The command line version is more convenient for debugging the source code and the rule base. The xview version is the final version, since it includes a graphical user interface (refer to chapter 5 in [13]).

5.1 Top level structure

As shown in the top level architecture of Fig 5.1, MOSAA has two kinds of user input files:

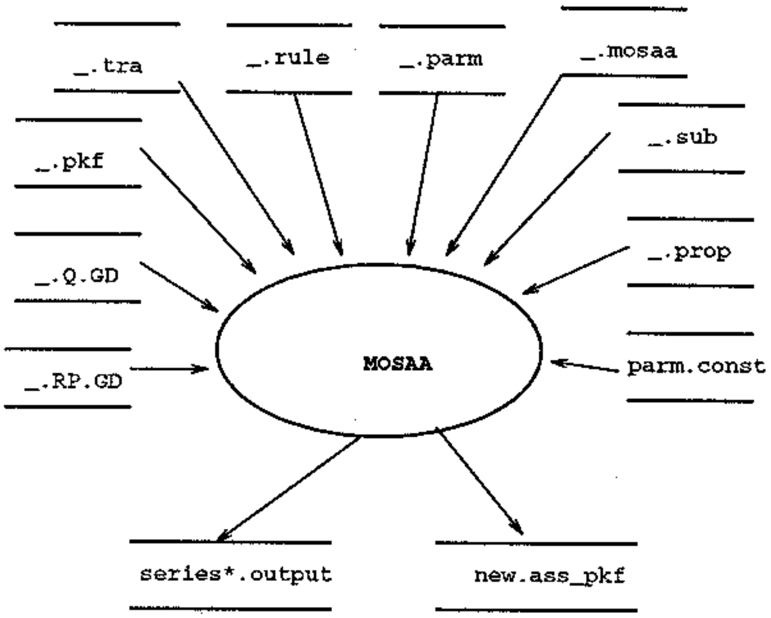


Figure 5.1: MOSAA top level user's perspective.

- Spectroscopy files -

  _.tra Spectrum plot file, used for graphically displaying the spectrum.

  _.pkf Peak finder file, data for assignment manipulation, also used for graphically displaying the "stick" spectrum.

  _.Q.GD calculated R-Q combination difference file.

  _.RP.GD calculated R-P combination difference file.

  Section 5.2 in [13] gives more details about these input files.

- Knowledge base files (Refer to Appendix B in [13])

  _.rule contains all the rules in different groups.

  _.parm contains the definitions of all the parameters used in the rules.

  _.mosaa contains the definitions of all the MOSAA functions used in the rules.

  _.sub contains the definitions of all the subroutines used in the rules.

_prop contains the definitions of all the properties used in the rules

parm.const constant parameters' values.

There are two kinds of output files:

- A group of files (e.g. Series0.output) which records the assigned series information. Each file contains one new assigned series. Chapter 6 gives an example of such output files.

- File `new.ass_pkf` is a copy of the peak finder file containing additional assignment information. When a peak is assigned, it has some additional information such as which series it belongs to and overlap situations. This file could be read in as a peak finder file, which gives more information for new series assignment.

The conventions of file names here are: 1) a leading ‘_’ character means the user provides one name for each file type; 2) an ‘*’ means one or more names.

The MOSAA system architecture from a developer's perspective is shown in Fig 5.2.

There are a total of 25,740 lines of source code in the command line version and a total of 28,390 lines of source code in xview version. This includes all *.h, *.cc and bison input files. It does not include the *.c and *.h files generated by lex and yacc. All of the source files for building MOSAA are in anonymous ftp site

```
physi02.novlab.unb.ca/pub/mosaa/command (command line version)
              "            /xview   (xview version)
              "            /input-file (input files)
```

5.2 Preprocessing

Before running the inference engine, some preprocessing must be done. Preprocessing includes defining input files, setting up the working environment and building the user interface.

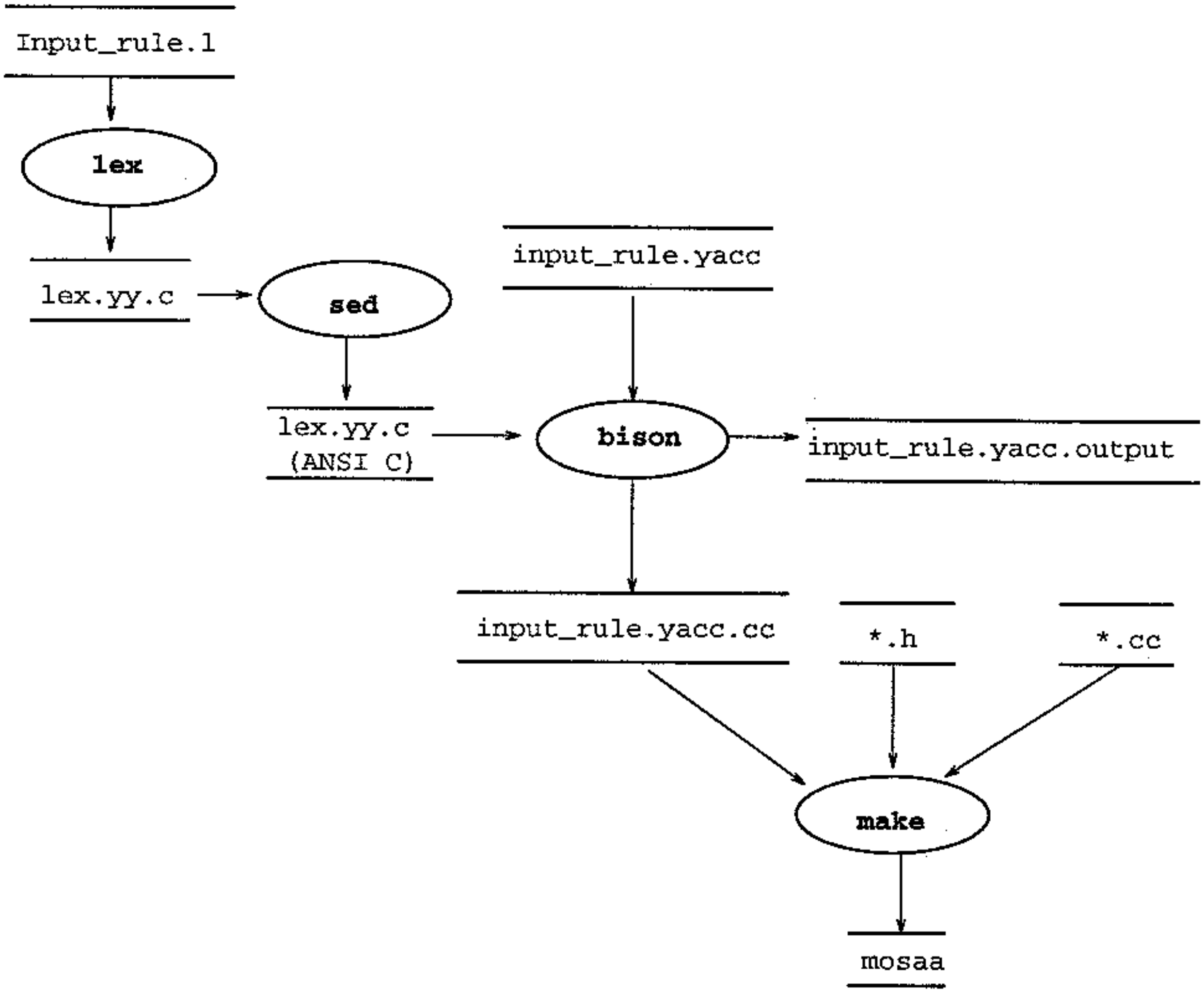


Figure 5.2: MOSAA top level developer's perspective.

5.2.1 Input Files

Rules in MOSAA are written in plain ASCII characters and contained in the `_.rule` file. This file is read in during preprocessing, and rules are compiled into an internal rule structure. Too add, remove or modify a rule, the ASCII `_.rule` file is edited appropriately.

Due to the complexity of the rule grammar, the compiler used to read in rules was produced by lexical analyzer *lex* and parser generator *bison* [8,18].

Appendix A in [13] gives the complete lex file `input_rule.l`, which is used to produce the lexical analyzer.

The grammar of MOSAA rules uses the grammar syntax of *bison*, which is essentially a machine-readable Backus-Naur format (BNF) [8]. The complete MOSAA rule grammar in bison syntax notation is described in shown in Appendix A.

All the parameters, MOSAA functions, subroutines, and properties must be defined in the files `_.parm`, `_.mosaa`, `_.sub` and `_.prop`, respectively. These files give sufficient information for later rule compiling and the running of the inference engine.

Chapter 2 in [13] gives the complete grammar of these files.

Several parameters' values are known initially and are put in the file `parm.const`, which is read into working memory during preprocessing.

Spectroscopy files, including the Peakfinder file, the spectrum file and the R-P, R-Q calculated combination difference files are also read in during preprocessing (see section 5.2 in [13]).

5.2.2 Zone classification

As mentioned in section 2.3, to pick the second line according the first line, one needs to know the approximate spacing between these two lines. If we already know 2B", which is close to the approximate spacing between two neighboring lines of one series in the low J case, we could use it to pick the second line. Otherwise, when the

R,P,Q pattern is clear, which means there are clear multiplets in the spectrum, we could try to find the approximate spacing between two neighboring multiplets during preprocessing.

Zone classification is used for this purpose. Zones, which we used instead of multiplets, refer to areas in the spectrum where strong lines are congested. Lines in the Peakfinder file are sorted first by their intensities. The top 300[1] strongest lines are resorted by their wavenumber. Zones are determined by scanning these lines according to their congestion. When the distance between two lines is small enough, they are in the same zone; otherwise, a new zone starts. Thus, we can define the range of each zone, and therefore calculate the approximate spacing between two neighboring zones.

This classification is normally correct in zones that have quite a few strong lines, which usually are multiplets with a J value not too low and not too high. Since the first line of the "Three Line Group" usually won't be picked in the case where J is too low[2], the approximate spacing we use for picking the second line is fairly good.

5.3 User interface

The user interface is very important in the MOSAA system. A lot of information is obtained from the user interactively.

In the MOSAA xview version, a user can view the Peakfinder file or the rule file. Two spectra are displayed with different resolutions[3] in two separated windows; each resolution can be adjusted by the user. The spectrum combines data from both the Peakfinder file and the Spectrum file, which are used for displaying the 'stick' spectrum and the real spectrum, respectively. The real spectrum is used only for display purposes, while the 'stick' spectrum is used for user interaction.

---

[1] Depending on the spectrum, we could use other numbers as well.

[2] As section 2.1.2 mentioned, the first line should be picked in a low J but strong enough multiplet, so this won't be where J is too low.

[3] 'resolution' used here refers to 'unit' shown in wavenumber, which is different from the normal computer science concept.

Fig 5.3 and Fig 5.4 show two pieces of a spectrum with different resolutions.

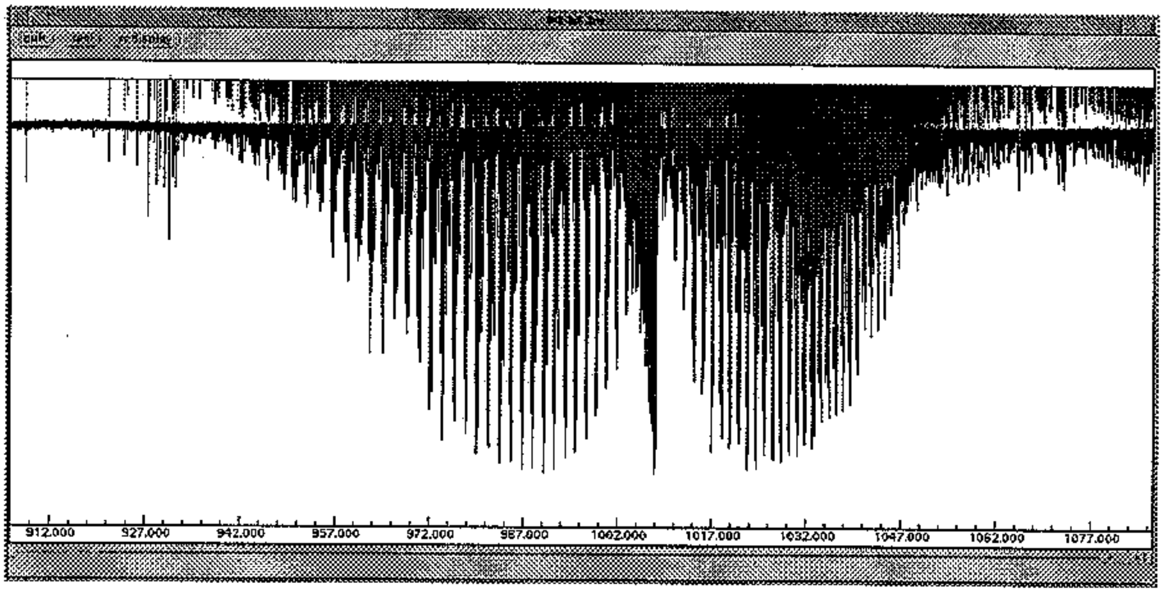


Figure 5.3: Low resolution spectrum of $CH_3^{18}OH$ in the 900-1100 cm^{-1} region.

A user can click on the spectrum to choose a required peak, as well as to add a missed peak. The dynamic series assignment process is shown in the spectrum by using different colours for sticks in the spectrum. Appendix D shows a piece of such a spectrum. Three colors appear in this spectrum. Blue lines are normal peaks in the peakfinder file. Red lines represent the peaks already assigned. A green line is the peak currently being searched during the assignment processing. When the system needs the user to make a decision, such as selecting one line from two candidates, the spectrum is scrolled to the corresponding region.

A special window is used for helping the user make decisions at some stages; Fig 5.5 shows a part of this window. As we can see, the spectrum is cut in segments according to already found lines in the current series. The lines that belong the same series lie in an almost vertical line. The idea of showing the spectrum in this way comes from the LOOMIS-WOOD program introduced in section 2.4.2.

Although the graphical user interface was built using X-windows(XView) programming, there is one concept that needs explanation.

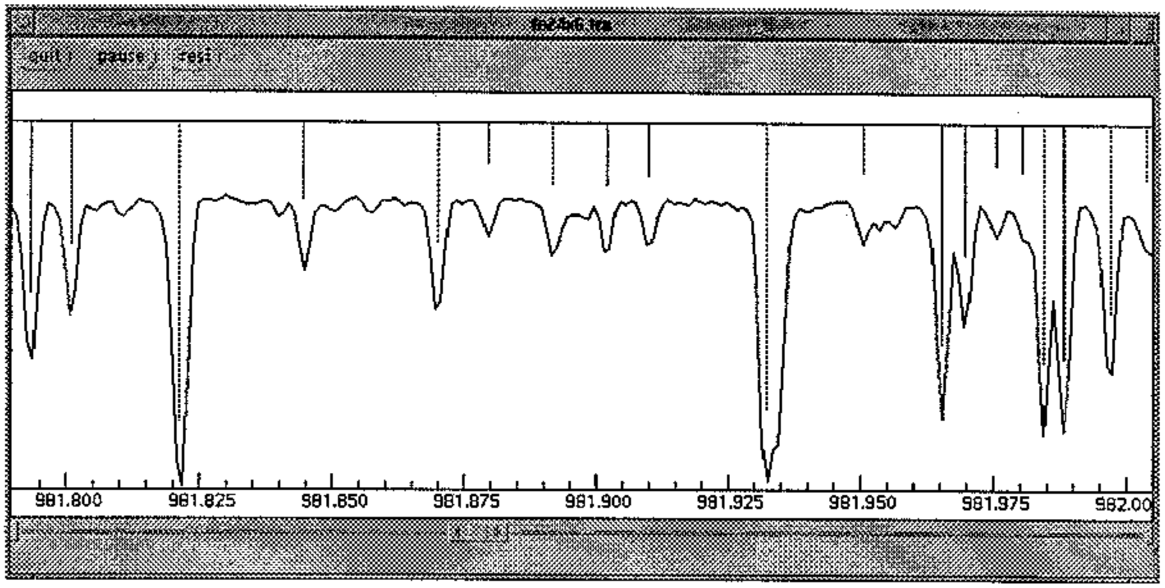


Figure 5.4: High resolution spectrum of $CH_3^{18}OH$ in the 900-1100 cm^{-1} region.

Window applications usually are event driven; since `mosaa` basically is run by the inference engine, it is mainline driven [24]. Instead of using `xv_main_loop`, we use:

```
while (!finished)
  {
    notify_dispatch();
    XFlush(main_dpy);
    if (start_assign==1)
       assign();
  }
```

`assign()` is a function that drives the whole inference engine, which invokes a lot of user interactive functions. If we put `assign()` into a callback, the events won't be dispatched until the callback returns. This is not convenient for an interactive interface. When the function `assign` is not a callback, we can put `notify_dispatch` in any place (except in the call back) to explicitly dispatch the event. This is very

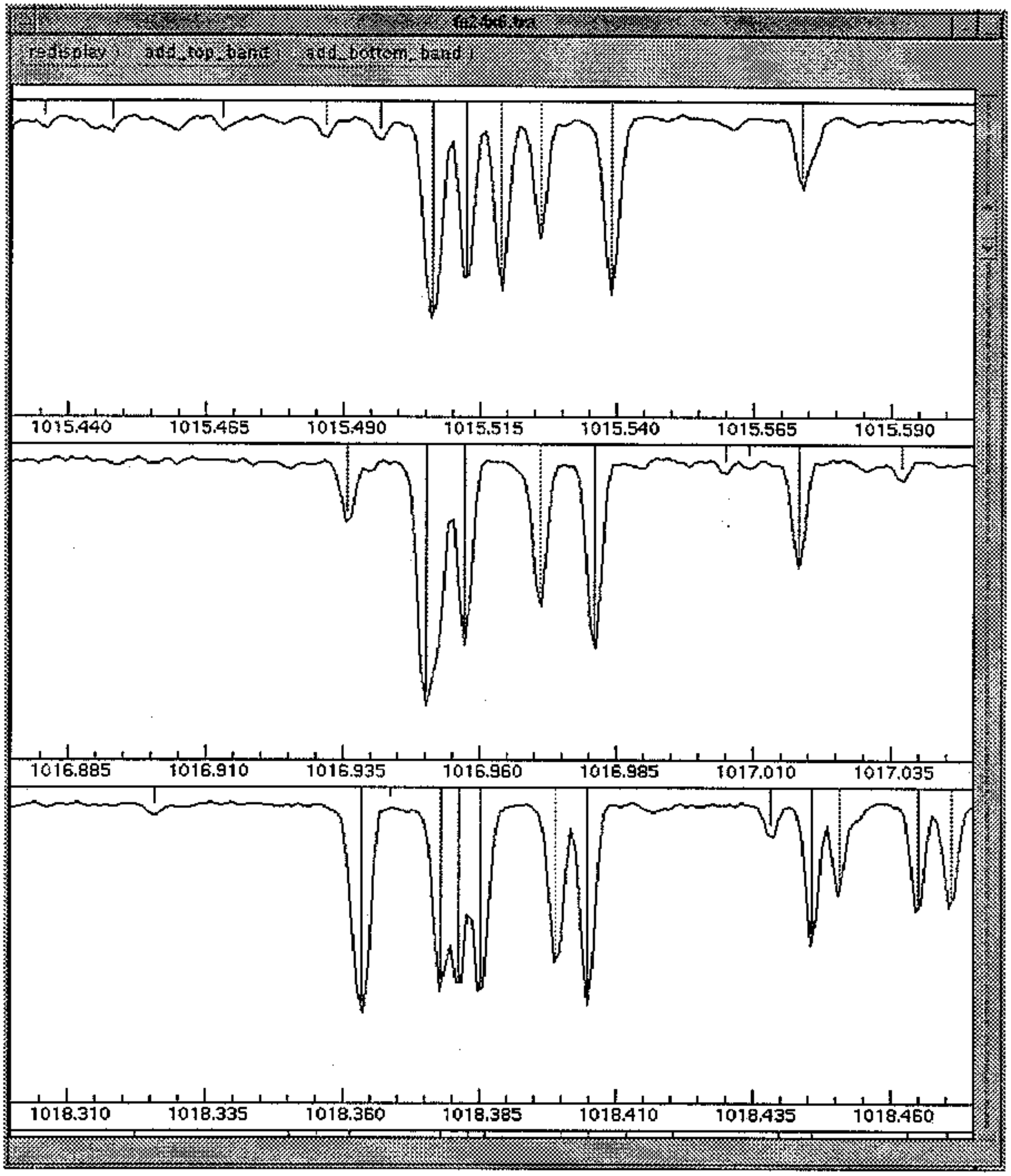


Figure 5.5: A piece of a zone sliced spectrum in Loomis-Wood format.

convenient since `mosaa` basically is a mainline driven program. For further information about X-windows/XView programming, please refer to an xview programming reference book, e.g. [24].

Chapter 6

Testing

The spectrum of $CH_3^{18}OH$ in the 900-1100 cm^{-1} region and the spectrum of $CD_3^{16}OH$ in the 910-1300 cm^{-1} region were used for testing purposes.

The spectrum of $CH_3^{18}OH$ was already assigned by experienced physicists and the output series information was obtained from several spreadsheet files (see Appendix B.1). This spectrum has been used ever since the start of the MOSAA implementation. When the inference engine and the rule base later became fairly stable, this spectrum was primarily used for testing and expanding the rule base.

The spectrum of CD_3OH in the 910-1300 cm^{-1} region was only used in the testing period, and had not previously been completely assigned by a physicist.

6.1 Testing of the spectrum of $CH_3^{18}OH$ in the 900-1100 cm^{-1} region testing

6.1.1 A sample process of assigning one series

The (035)E2 series is picked here for explaining the MOSAA series assignment process.

All the major processing[1] is shown on the CRT during MOSAA running. A complete record of this displayed output can also be captured using a '`typescript`' file. Appendix B.2 shows some pieces abstracted from the typescript file which records the (035)E2 series assignment process. The main window of the xview version of MOSAA is shown in Fig 6.1. Before the assignment starts, several files must be loaded and the preprocessing must be done. The user is then prompted to pick the first line of the "Three Line Group". Line 1027.861745 was picked as the first line in this example.

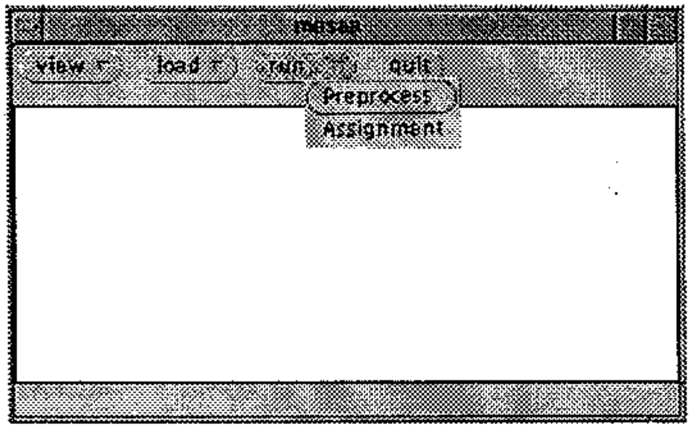


Figure 6.1: The main window in MOSAA xview version.

The inference engine then searches for a "Three Line Group" according to this first line using the technique mentioned in section 2.3. The first combination of three lines which may generate a series is as shown in Fig 6.2. To search for the fourth line, there are two candidates, line 1031.847028 and line 1031.842037. The inference engine can't find proper rules to handle this case [2], so it asks the user to pick one as shown in Fig 6.2. Both choices here for the fourth line are equally likely, with comparable anomalies in the second difference $\Delta 2$ and the intensities. Thus, the user would probably have to try both choices to see if further lines would shed light on the series trend.

---

[1] Includes the deduction paths of rules, all important decisions made as well as some debugging information

[2] which makes this case confusing in the manual assignment process also

```
** Do select_bottom_line( , 5178, , 5177, , )

choice 1:
The candidate is from down extracting
 SpreadSheet is:
 R,
parm=Cur_Peaks[15].J,  has_J=0
Index    J        wv          delta1      delta2      intens
15.            1027.861745  1.348672                 0.383996
16.            1029.210417  1.327538   -0.021134   0.660026
17.            1030.537955  1.309073   -0.018465   0.533268
18.            1031.847028                           0.301236

choice 2:
The candidate is from down extracting
 SpreadSheet is:
 R,
parm=Cur_Peaks[15].J,  has_J=0
Index    J        wv          delta1      delta2      intens
15.            1027.861745  1.348672                 0.383996
16.            1029.210417  1.327538   -0.021134   0.660026
17.            1030.537955  1.304082   -0.023456   0.533268
18.            1031.842037                           0.264357

Please pick one (1,  2,  or 0-none of them):
2
```

Figure 6.2: A sample part of MOSAA processing requesting user input after showing the current "Three Line Group" (take from part A of Appendix B.2).

```
 SpreadSheet is:
 R,
parm=Cur_Peaks[7].J,  has_J=0
Index    J        wv          delta1       delta2     intens
 7.            1016.935647  1.427823                  0.752472
 8.            1018.363470  1.407774    -0.020049    0.223020
 9.            1019.771244  1.391835    -0.015939    0.538795
10.            1021.163079  1.374718    -0.017117    0.463053
11.            1022.537797  1.357109    -0.017609    0.391154
12.            1023.894906  1.336639    -0.020470    0.384100
13.            1025.231545  1.321518    -0.015121    0.538079
14.            1026.553063  1.308682    -0.012836    0.189987
15.            1027.861745  1.294771    -0.013911    0.383996
16.            1029.156516  1.280764    -0.014007    0.565841
17.            1030.437280                            0.267685

** Do select_modify_type( )
add line ------- a
modify line ---- m
delete line ---- d
no operation --- n
Add a missed peak into .pkf file --- p
Change CD type --- c
This series is totally wrong, quit --- q
```

Figure 6.3: A sample showing part of MOSAA processing when a series candidate is found, and the user needs to make a corresponding decision (from part B of Appendix B.2).

A variety of such interactive means to get information while the inference engine is running are used by MOSAA. As more and more rules are added into the rule base, more cases can be handled by rules instead of requiring interactive methods. MOSAA was designed to allow this knowledge base expansion to occur.

When no more lines can be found in the R branch of the current series, up and down searching terminates. The current series information is then displayed in spreadsheet format as shown in Fig 6.3.

The user can decide whether the found series is acceptable or not by checking this spreadsheet as well as the zone sliced spectrum in Loomis-Wood format[3] in the user interface. If it is not accepted, the inference engine will go back to a certain point to restart searching. Otherwise, the inference engine starts searching for the corresponding P branch using the current R branch.

Commencing with the four successive lines around the first line in the R branch[4], the corresponding four lines in the P branch are searched for, and the RPQ confirmation is done if possible. If four lines can't be found, there could be some problems: the R branch found is not correct, the calculated R-P combination differences are not good enough, overlap or perturbation is affecting one or more of the four lines in the R branch or the P branch, or possibly the rules themselves are not good enough. Currently, the inference engine just goes back to restart searching the R branch from a certain point. More rules could be added here to deal with different situations.

When four lines in the P branch are found and the extraction of the P branch is done, the inference engine goes back to search the R branch according to the currently found P branch. Then the inference engine searches from the R branch to the P branch and from the P branch to the R branch again as long as new lines can still be found. Using this back and forth method, more lines can be found, and more corrections can be done.

During the process, the user can get a chance to solve several problems, such as inserting lines missing from the peak finder file, which is encountered frequently in the P branch and in weak line areas. Users can change their mind when the wrong selection has been made. For instance, in the case shown in Fig 6.4 (part C of Appendix B.2), the user may pick line `1042.132853`[5]. Later if the user feels this is not correct, 'm' can be entered when the menu shown in Fig 6.3 pops up. Another line can be picked and the inference engine will restart the up and down searching process. There are some

---

[3] As shown in Fig 5.5.

[4] These four lines can be any four successive lines as long as they include the first line picked by the user.

[5] Although normally line `1042.140355` will be picked by a reasonable $\Delta 2$.

other methods to allow the user to control the process, doing some modifications as shown in the menu of Fig 6.3. These interactive methods will always be necessary even when the rule base is very powerful due to the complexity of spectroscopic assignment.

The Q branch is also searched during the process of searching for the R and P branches. So far, it is difficult to confirm Q branch lines due to the high congestion in the Q branch in this band.

When all the work has been done for the current series, two output files are written. The information on the current series is exported into the file `seriesx.out`, which is as shown in Appendix B.3. Users can also output useful information into the file `new.ass_pkf` as shown in Fig 6.5.

Basically, `new.ass_pkf` is a copy of the peak finder file with the assigned line information added. Peak '`1 CO 0 0 5 E2 R 7 c`' shows the following assigned information of peak `1019.771244`:

assigned	band_name	n	τ[6]	K	asymmetry	branch	J	comments
1	CO	0	0	5	E2	R	7	c

Additional information usually can be put in the comments part; e.g. 'c' means this peak assignment has been RPQ confirmed and 'o' means the peak is overlapped. Notice that peak `1019.809931` has two blocks of information associated with it, since this peak is overlapped. So we know peak `1019.809931` belongs to two series.

The `new.ass_pkf` file can be used as input to MOSAA next time for assigning the next series. It also helps in the graphical interface, since lines which are already assigned are displayed with a certain color, and this helps the user make further decisions.

The output for this (035)E2 series was compared with the spreadsheet file prepared by hand (Appendix B.1). Lines R(5) to R(31) are the same, where as Lines R(32) to R(35) are not found by MOSAA. The reason is that R(32)-1049.274108 is missed in

---

[6] τ value here is temporary using '0'. In fact the τ value can be obtained from the n and K values; this function can be implemented easily using a lookup table in the future.

```
** Do select_bottom_line(  , 6076,  , 6075,  , )

choice 1:
The candidate is from down extracting
 SpreadSheet is:
 R,
parm=Cur_Peaks[7].J,  has_J=0
Index     J        wv          delta1       delta2      intens
 7.             1016.935647  1.427823                   0.752472
 8.             1018.363470  1.407774    -0.020049     0.223020
 9.             1019.771244  1.391835    -0.015939     0.538795
10.             1021.163079  1.374718    -0.017117     0.463053
11.             1022.537797  1.357109    -0.017609     0.391154
12.             1023.894906  1.339657    -0.017452     0.384100
13.             1025.234563  1.322407    -0.017250     0.388059
14.             1026.556970  1.304775    -0.017632     0.385661
15.             1027.861745  1.287316    -0.017459     0.383996
16.             1029.149061  1.269753    -0.017563     0.391489
17.             1030.418814  1.252379    -0.017374     0.412323
18.             1031.671193  1.234256    -0.018123     0.292232
19.             1032.905449  1.216726    -0.017530     0.437019
20.             1034.122175  1.199070    -0.017656     0.461675
21.             1035.321245  1.181244    -0.017826     0.463786
22.             1036.502489  1.163292    -0.017952     0.495581
23.             1037.665781  1.145341    -0.017951     0.566984
24.             1038.811122  1.128060    -0.017281     0.591718
25.             1039.939182  1.109391    -0.018669     0.358014
26.             1041.048573  1.091782    -0.017609     0.673768
27.             1042.140355                            0.707450

choice 2:
The candidate is from down extracting
 SpreadSheet is:
 R,
parm=Cur_Peaks[7].J,  has_J=0
Index     J        wv          delta1       delta2      intens
 7.             1016.935647  1.427823                   0.752472
 8.             1018.363470  1.407774    -0.020049     0.223020
```

Figure 6.4: A sample part of MOSAA processing requesting user to choose one of the lines during line down searching.

9.	1019.771244	1.391835	-0.015939	0.538795
10.	1021.163079	1.374718	-0.017117	0.463053
11.	1022.537797	1.357109	-0.017609	0.391154
12.	1023.894906	1.339657	-0.017452	0.384100
13.	1025.234563	1.322407	-0.017250	0.388059
14.	1026.556970	1.304775	-0.017632	0.385661
15.	1027.861745	1.287316	-0.017459	0.383996
16.	1029.149061	1.269753	-0.017563	0.391489
17.	1030.418814	1.252379	-0.017374	0.412323
18.	1031.671193	1.234256	-0.018123	0.292232
19.	1032.905449	1.216726	-0.017530	0.437019
20.	1034.122175	1.199070	-0.017656	0.461675
21.	1035.321245	1.181244	-0.017826	0.463786
22.	1036.502489	1.163292	-0.017952	0.495581
23.	1037.665781	1.145341	-0.017951	0.566984
24.	1038.811122	1.128060	-0.017281	0.591718
25.	1039.939182	1.109391	-0.018669	0.358014
26.	1041.048573	1.084280	-0.025111	0.673768
27.	1042.132853			0.624209

Fig 6.4 (continued)

the peakfinder file. The user could add this line to the peak finder file by displaying the appropriate section of the spectrum on the screen and clicking on the missing line[7]. Lines P(6) to P(34) are the same, where as Line P(5) picked by the program is not a part of the series, and the user could ignore this line. The results in the Q branch are not as good as in the R and P branches due to the high congestion in the Q branch. Q(7) to Q(18) are assigned by MOSAA in the same way as done by hand. Lines Q(5), Q(6) and Q(19) to Q(27) are discovered by hand, but not by MOSAA.

6.1.2 Other series assignment in this region

Trials were conducted for several other series in the $CH_3^{18}OH$ spectrum. The 'E' series are easier to assign than the 'A' series due to the splitting in the 'A' series.

---

[7] Checking the zone sliced spectrum in Loomis-Wood format as shown in Table 5.5 can be a great help

```
1019.760155      0.228791
1019.765076      0.986391
1019.771244      0.538795 1 CO 0 0 5 E2 R 7 c
1019.787987      0.268836
1019.792861      0.249195
1019.795973      0.250349
1019.809931      0.095409 1 CO 0 0 3 E2 R 7      1 CO 0 0 0 E1 R 7 o
1019.814797      0.958477
1019.821839      0.815749
1019.830285      0.633906
1019.849632      0.550851
1019.855691      0.401719 1 CO 0 0 4 E1 R 7 c
1019.872925      0.947464
```

Figure 6.5: A piece of file new.ass_pkf.

Results for the tested series are in Appendix B.3; they are relatively good comparing the MOSAA results to the manually generated spreadsheet as shown in Table 6.1.

However, MOSAA was not successful with some of the series picked for testing. One example is (012)E2 shown in Appendix B.5. Although the R branch is found and is quite good (R(6) through R(36) are correct), the corresponding P branch can't be found due to the high bias in the calculated R-P Combination differences. This is one of the main problems causing the failure of the assignment. Another example is (032)E2 shown in Appendix B.5. R(2) through R(44) are correct, but RPQ confirmation for the 'Three Line Group' couldn't be done since there are not enough Q lines. The failure of doing RPQ confirmation[8] for the 'Three Line Group' is another main problem causing the failure of this assignment. Some other problems are due to the overlap and perturbation as mentioned in Chapter 2. These problems could be solved later by improving the quality of the calculated R-P combination differences. Enlarging the RPQ confirmation error tolerance or getting rid of the RPQ confirmation can let the

---

[8] RPQ confirmation is very necessary for assigning the spectrum which doesn't have high quality calculated R-P combination differences. So we shouldn't get rid of the RPQ confirmation process for this spectrum.

Table 6.1: The comparison of the lines assigned by MOSAA with the lines assigned manually prepared in the spectrum $CH_3^{18}OH$ in the 900-1100 cm^{-1} region.

Series	manually			MOSAA		
	R	P	Q	R	P	Q
(010)A	0-42	1-39		0-37	1-36	
(011)E2	1-37	2-39	1-4	1-36	2-38	2-4
(013)A+	3-41	4-37	3-15	3-25	4-27	3-12
(013)A-	3-35	4-37	3-15	3-33	4-36	3-13
(015)E1	5-35	6-37	5-24	5-34	6-34	8-14
(016)A	6-38	7-38	6-31	6-35	7-35	7-28
(023)E2	3-39	4-39	3-18	3-37	4-36	8-16
(024)E1	4-38	5-38	4-16	4-27	5-37	5-14
(026)E2	6-33	7-36	6-29	6-30	7-34	11-17
(030)E	0-38	1-38		0-37	2-36	
(035)E2	5-35	6-36	5-27	5-31	6-34	5-18

P branch be found, but one must be more careful since a wrong P branch may be picked.

The constant values set in the constant parameter file parm.const also affect the outcome. For instance, constant parameter RPQ_CONFIRM_ET defines the error tolerance of RPQ confirmation as mentioned in section 2.3. If this value is set too large, some incorrect RPQ sets could erroneously be classified as confirmed. If the value is set too small, the RPQ confirmation will be limited and this may cause a problem in obtaining the first four P lines in the initial transfer from the R branch to the P branch. The values for the constant parameters vary a lot from one spectrum to another spectrum, due to different molecules, species and bands. This will be mentioned more in the next section.

6.2 Spectrum $CD_3^{16}OH$ in 915-1030 cm^{-1} region testing

The spectrum of $CD_3^{16}OH$ in the 915-1030 cm^{-1} region was used just for MOSAA testing. This spectrum is still relatively unexplored and during the initial testing, no assigned lines spreadsheets were used for comparison.

First of all, the constant parameter file `parm.const` was adapted to this new region. Most of the parameters such as `ERROR_TOLERANCE` could be set to the same values as in `parm.const` for the first spectrum tested in section 6.1. Some of the parameters, such as parameter `ROUGH_2B` had to be modified. Since the assignment for this series was started from scratch, these values were set initially by looking at the spectrum and by previous assignment experience. Table 6.2 shows the values of the constant parameters in the `parm.const` for the spectrum of $CH_3^{18}OH$ in the 900-1100 cm^{-1} region and the spectrum of $CD_3^{16}OH$ in the 910-1300 cm^{-1} region.

The testing is focused on previously unexplored n=1 spectral regions, in which the lines are spread out and are relatively weak compared to the n=0 regions. As shown in Fig 6.6, the n=0 region occurs between around 952.390 - 952.660, and the n=1 region occurs after around 952.660.

Several series were assigned and the corresponding results are in Appendix C.2[9], [10].

The results for this test were much better than the first test using the spectrum $CH_3^{18}OH$ in the 900-1100 cm^{-1} region. The main reason is that the R-P combination differences used here[11] are much more accurate than the calculated R-P differences

---

[9] Later, some of the series assignments were checked independently by Dr. R.M.Lees. These spreadsheet files are in Appendix C.1.

[10] The output of this testing is a little bit different from the first testing. There is one extra column; i.e. the observed R-P difference for each series spreadsheet. This is added in after the first testing which helps in choosing the right P branch when there are several possibilities.

[11] The R-P combination differences used here are calculated from energy levels which are calculated from global fit[19].

Table 6.2: The values of the constant parameters in the `parm.const` for the spectrum of $CH_3^{18}OH$ in the 900-1100 cm^{-1} region and the spectrum of $CD_3^{16}OH$ in the 910-1300 cm^{-1} region.

parameter	$CH_3^{18}OH$	$CD_3^{16}OH$
INTENS_ADJUST_LIMIT	0.1	0.1
CLOSE_DEFI	0.15	0.15
ERROR_TOLERANCE	0.001	0.001
FAR_MORE_DEFI	4	4
FEW_Q_K	0	2
I_EXT	0.3	0.3
I_EXT_FOR_WEAK_PEAK	0.2	0.2
MAX_DELTA2	0.03	0.01
MAX_SERIES_NUM	50	50
MAX_BIAS	0.006	0.006
MINI_DELTA2	0.01	0.003
MINI_S_L_NUM	10	10
RESL	0.002	0.002
S_RANGE1	0.2	0.2
SEARCH_EXT1	20	20
SEARCH_WV_EXT	0.01	0.01
STRONG_PEAK_INTENS	0.35	0.35
ROUGH_2B	1.4	1.25
R_P_MATCH_ET	0.001	0.0003
R_P_MATCH_ET_MIN	0.0003	0.0003
R_P_MATCH_ET_MAX	0.003	0.002
R_P_MATCH_ET_STEP	0.001	0.0002
R_Q_MATCH_ET	0.003	0.003
RPQ_CONFIRM_ET	0.002	0.002
R_P_INTENS_DIFF	0.4	0.4
TOO_STRONG_PEAK_INTENS	0.1	0.1

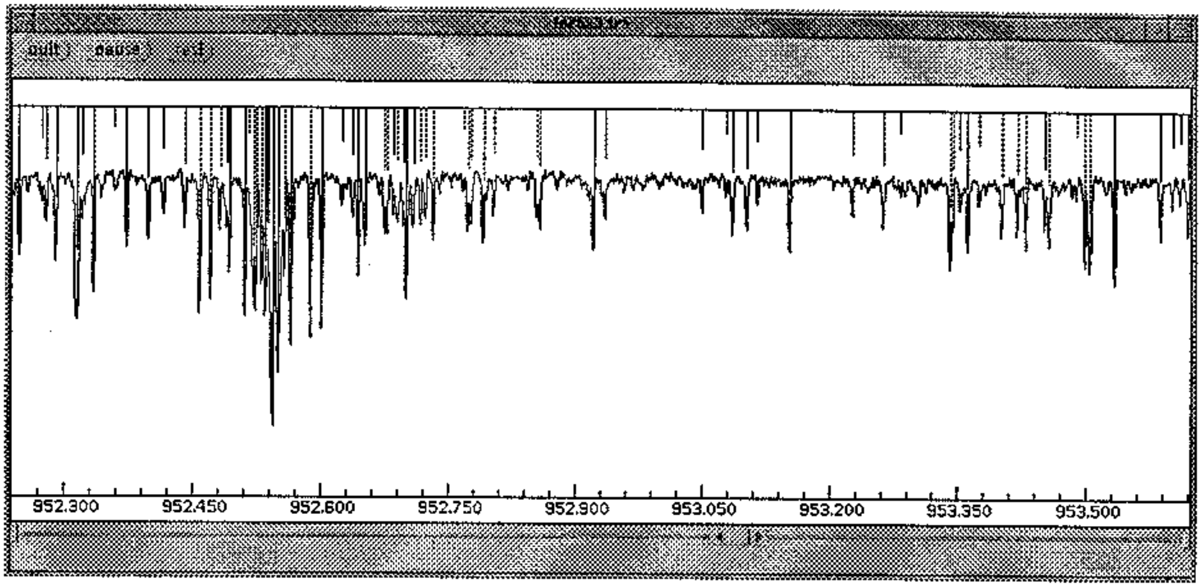


Figure 6.6: A piece of spectrum of $CD_3^{16}OH$ in 915-1030 cm^{-1} region.

used in the first testing[12]. Another factor is that this testing is focused on the n=1 region, where the lines are not as congested as lines in the n=0 region. This leads to fewer overlap cases for the n=1 region. Table 6.3 shows the comparison of the MOSAA results to the manually generated spreadsheet.

One problem discovered in this testing is that for several series, the R branch lines found were good, while no P branch lines could initially be found. Series (133)E1 is one example, where the R branch found is perfect, but no P branch could be found. This is due to J-shifting of this series in the spectrum. According to rule `C_R32`, line `994.106180` should have had a J value of 4 or 5[13]. In fact, the J value for this line is 6 because the whole (133)E1 series is down-shifted in the spectrum relative to its neighboring series. To fix this problem, rule `C_R32` was modified to extend the range of J values to try. This then gave the good result as shown in Appendix C.2. The range of J to try can be as large as we want, as long as time and computer memory

---

[12] Because of the high quality of R-P combination differences of this spectrum, RPQ confirmation is not strictly required.

[13] Even by looking at the spectrum, most probably we also will get the same assumption.

Table 6.3: The comparison of the lines assigned by MOSAA with the lines assigned manually prepared in the spectrum $CD_3^{16}OH$ in 915-1030 cm^{-1} region.

Series	manually			MOSAA		
	R	P	Q	R	P	Q
(010)A	0-35	1-32		0-19	1-31	
(030)E	0-26	1-27		0-26	3-24	
(121)E1	1-32	3-33	1-40	1-22	4-19	
(124)E1	4-21	5-21	4-18	4-21	5-21	5-18
(125)A	5-24	6-29	5-40	5-24	6-29	6-17
(130)E1	0-30	1-30		4-30	1-29	
(132)E2	2-26	3-28		3-23	3-28	
(133)E1	3-33	4-33	3-40	3-33	4-33	3-13
(131)A+	2-29	2-30	1-29	2-29	2-23	
(131)A-	2-29	2-30	1-29	2-29	2-23	
(134)A	4-32	5-31	4-19	4-28	5-31	4-11

allow. This is good for assigning more widely spread spectra in which a lot of lines are shifted and the assumptions for J values are difficult to predict. For methanol, for example, this situation applies to the methyl-rocking infrared bands for which the different series are reported to be spread over an interval of about 5 cm^{-1} so the J values are correspondingly spread out [23,25,26].

6.3 Assessment of Results

When methanol spectra are assigned by hand, several hours (usually 2-3) per series are required to enter data in spreadsheets and cross-check against spectra. MOSAA takes an average of about 15-30 miniutes for assigning a series[14]. Several factors can affect the time taken by MOSAA. When a series is J-shifting, MOSAA runs much longer trying to get the right J value. The user assistance, and quality of the spectrum[15] also affects the performance of MOSAA. Certainly the speed of CPU and the memory of

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[14] This doesn't include the unsuccessful cases. Time used for error checking afterwards is not included.

[15] Which means if the spectrum is highly congested or not; if the R-P combination difference sets are good or not etc.

the computer are also very important.

MOSAA enhances the effectiveness of the spectroscopist to spend time being an expert rather than just doing routine work. Spectroscopists can be relieved from housekeeping; they can focus on trouble spots and new things, thus time is usefully spent at more difficult problems. The normal routine work in methanol spectroscopic assignment is '*trial and error*', and this is exactly what MOSAA does. The graphical interface is also a help for spectroscopists. When assignments run into a problem, the user can look at the zone sliced spectrum or different resolution spectrums, instead of looking at the physical spectrum itself.

One important aspect in using MOSAA is updating a spectrum. The spectroscopist often repeats a spectrum recording with different experimental conditions, hence automated updating of the assignments using the new peak finder file will be very much faster with MOSAA, while manual operation is almost as long as for the original spectrum.

Chapter 7

Conclusions and Future work

7.1 Conclusions

The main emphasis of this thesis was on developing a knowledge-based system (MOSAA) to assist physicists or other scientists in the assignment of peaks in molecular spectra. MOSAA's inputs include the molecular spectral information, and a knowledge base containing known energy levels and constants for the given molecules, and rules provided by an expert for performing the assignment.

Two basic components of MOSAA are the knowledge base and the inference engine. The knowledge base here contains knowledge of methanol spectroscopic assignment, which is represented by rules together with their associated components (parameters, functions and properties) written in the MOSAA grammar. The MOSAA grammar was specifically designed to accommodate knowledge about molecular spectroscopic assignment. MOSAA rules are categorized into three groups: G-Goal, C-Consequence and A-Antecedent rules. There are four different kinds of parameters used for different purposes, as well as two types of functions. Several processes used in methanol spectroscopic assignment can be accomplished using functions embedded in a rule. The premises and the conclusions of rules can have different formats, such as single parameter, MOSAA function, subroutine, or a loop. Different rule properties such as `TRY`, `Restart` and `MATCH` are very helpful in translating some special spectroscopic assignment techniques into rules. A total of 313 rules were written for the current version of MOSAA. Using these properties, the rules can be written in a very flexible and powerful way.

The MOSAA inference engine combines backward chaining and forward chaining, as well as two special mechanisms 'TRY' and 'Restart'. These two special mechanisms are designed to control the inference engine running, and, in particular, to deal with methanol spectroscopic assignment searching. A history tree, working memory, working memory store as well as a try store are used for implementing the inference engine. The inference engine was written using C++.

Two versions of MOSAA were developed; the *command line* version and the *xview* version. The *xview* version includes a graphical user interface, which allows the user to view the peakfinder file or the rule file. Two spectra are displayed with different resolutions in two separated windows. The user can click on the spectrum to choose a required peak. The dynamic series assignment process is shown in the spectrum using colored peaks. A special window which cuts the spectrum into segments aligned in Loomis-Wood spectroscopic format is used to help the user make decisions at various stages. This graphical user interface was built using X-windows(XView) programming.

The spectrum of $CH_3^{18}OH$ in the 900-1100 cm^{-1} region and the spectrum of $CD_3^{16}OH$ in the 915-1030 cm^{-1} region were used for testing. The series picked for testing are random, so they are representative of situations arising in the whole region. The results are relatively good compared to the previous manually assigned series stored in spreadsheets. The testing pointed out difficulties in computer-assisted spectroscopic assignment. Some of these difficulties were overcome by improving MOSAA rules; others were not overcome due to the complexity of the spectroscopic assignment process.

The results of testing of Spectrum $CD_3^{16}OH$ in the 915-1030 cm^{-1} region is better than testing of Spectrum $CH_3^{18}OH$ in 900-1100 cm^{-1} region due to the more accurate R-P combination differences used. The unsuccessful case met in the testing of Spectrum $CH_3^{18}OH$ in 900-1100 cm^{-1} region didn't appear in the Testing of Spectrum $CD_3^{16}OH$ in the 915-1030 cm^{-1} region[1].

7.2 Future work

Future work can be focused on two main parts; namely the explanation facility and the expansion of the knowledge base.

7.2.1 Explanation Facility

An explanation facility is commonly used in a knowledge based system. It can be very simple, or it also can show very detailed deduction information to the user. This facility is very useful to help the user understand the knowledge base (rules) and the processing mechanism provided by the inference engine.

The MOSAA system so far doesn't include an explanation facility. As was mentioned in 4.3, the history tree can be used for tracking the deduction process.

The fact base of MOSAA is working memory, which records current values of all known parameters. So the *fact* to be explained to the user is actually how the *parameter* is deduced. Thus, for each parameter in working memory, we could add one pointer, which points to a node in the history tree; the rule this node refers to is the one that most recently set the value of this parameter. Whenever a parameter is explained, its deduction could be found in the history tree and be displayed.

---

[1] Only one case was unsuccessful, which was due to line overlap instead of having a problem in R-P combination differences or RPQ confirmation.

7.2.2 Expansion of the Knowledge base

As mentioned in previous chapters, knowledge base expansion can be mainly classified into the following parts:

- Currently 65 processes in methanol spectroscopic assignment are done using functions embedded in a rule, which causes the information to be hidden. Some of the processes could be translated into rules in the future.

- As mentioned in chapter 6, several factors affect the correctness of the assignment results, such as overlapping and perturbation. More rules could be added into the rule base to solve these problems in the future.

- The knowledge base in this thesis contains the basic knowledge of methanol spectroscopic assignment. The testing carried out here was for the spectrum of $CH_3^{18}OH$ in the 900-1100 cm^{-1} region and the spectrum of $CD_3^{16}OH$ in the 915-1030 cm^{-1} region. In order to use MOSAA for other spectra, which could involve either different methanol species, different bands or different regions, more knowledge must be added into the knowledge base. Since the basic assignment techniques are the same, a modest number of rules need to be added, while the values of constant parameters need relatively more modifications.

- Rules in the rule base are based on the spectroscopic assignment techniques specifically adapted to methanol. The techniques used for other molecules may be similar to this, but might have substantial differences. To use MOSAA for doing assignments for some other molecules may need only minimal modification to expand the existing knowledge base, or may require building the whole knowledge base from scratch. Application of MOSAA to another molecular assignment domain remains to be investigated.

- Lines already assigned can be moved from the peak finder file, so these lines won't appear in the "stick" spectrum[2] in the screen. When more and more series are assigned, more and more "sticks" can be moved from the screen. This can help the user in picking the first line or making the decision when there are two choices. during MOSAA running.

---

[2] As mentioned in section 5.3, the spectrum displayed in the screen combines two parts: the real spectrum and the "stick" spectrum. The data in the peakfinder file are used for showing the "stick" spectrum. Each line in the peakfinder file corresponds to one "stick" in the "stick" spectrum.

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Appendix A

Grammar in bison syntax

The compiler used to read in the rules is produced by lexical analyzer *lex* and parser generator *bison* [8,18].

MOSAA rules' lexical convention is not given here; Appendix A in [13] gives the complete lex file `input_rule.l` which is used to produce the lexical analyzer.

Fig A.1 gives the grammar of MOSAA rules in the syntax notation of *bison*, which is *essentially a machine-readable* Backus-Naur format(BNF) [8].

This figure is abstracted from the auxiliary output file `y.output` of

```
yacc -v input_rule.yacc
```

The reason that we use the auxiliary output file of `yacc` instead of the `input_rule.yacc.output` from `bison` is that the syntax notation in `y.output` is closer to the context free notation of a rule grammar. Since both `input_rule.yacc.output` from `bison` and `y.output` from `yacc` are obtained from the grammar of `input_rule.yacc`, so there is no difference except the notation used.

The details of BNF and the grammar of *bison* are not given here; please refer to [7] for the description of BNF, and [8,18] for further information about *bison*.

The basic symbols used in Fig A.1 are listed in Table A.1. The last four rows in table are not used in the bison grammar; they are used in defining parameters and

```
Grammar
   0  $accept : begin $end
   1  begin : start
   2  start : rule_list
   3        | start rule_list
   4  rule_list : '%' CR c_ruleset
   5            | '%' GR ag_ruleset
   6            | '%' AR ag_ruleset
   7  c_ruleset : c_rule
   8            | c_ruleset c_rule
   9  c_rule : cr_ruleid IF premise THEN conclusion property comment
  10  cr_ruleid : CR
  11  premise : condition
  12          | premise '&' condition
  13  condition : loop
  14            | parm
  15            | subroutine
  16            | mosa_func
  17  loop : loop_type loop_var '=' loop_start ';'
                                   loop_end loop_step '{' loop_body '}'
  18  loop_var : LOOPI
  19           | LOOPD
  20  loop_type : FOR
  21            | ANYIF
  22            | DO
  23  loop_start : exp
  24  loop_end : exp
  25  loop_step :
  26            | ';' exp
  27  loop_body : condition
  28            | loop_body '&' condition
  29  parm : parm_name
  30       | parm_name '[' index ']'
  31       | parm_name '.' field
  32       | parm_name '[' index ']' '.' field
  33  index : INTEGER
  34        | LOOPI
  35        | parm
  36  parm_name : IDENTIFIER
  37  field : IDENTIFIER
```

Figure A.1: MOSAA rule grammar in bison syntax notation.

```
38  subroutine : ´$´ name ´(´ arglist ´)´
39             | ´$´ name ´(´ ´)´
40  mosa_func : mosa_name arglist
41            | mosa_name
42  mosa_name : MOSA_NAME
43            | ´=´
44  conclusion : conclu_condition
45             | conclusion ´&´ conclu_condition
46  conclu_condition : conclu_loop
47                   | subroutine
48                   | mosa_func
49  conclu_loop : loop_type loop_var ´=´ loop_start ´;´
              loop_end loop_step ´{´ conclu_loop_body ´}´
50  conclu_loop_body : conclu_condition
51                   | conclu_loop_body ´&´ conclu_condition
52  property :
53           | ´#´ prop
54  prop : prop_item
55       | prop ´&´ prop_item
56  prop_item : name
57            | name arglist
58            | name ´{´ conclusion ´}´
59  name : IDENTIFIER
60  comment :
61          | COMMENT
62  arglist : arg
63          | arglist ´,´ arg
64  arg : exp
65      | ´(´ arg_func ´)´
66  arg_func : mini_mosa_func
67           | mini_subroutine
68  mini_mosa_func : mosa_name explist
69                 | mosa_name
70  mini_subroutine : ´$´ name ´(´ explist ´)´
71                  | ´$´ name ´(´ ´)´
72  explist : exp
73          | explist ´,´ exp
```

Fig A.1 (continued)

```
exp : single_value
    | LOOPI
    | LOOPD
    | parm
    | exp '+' exp
    | exp '-' exp
    | exp '*' exp
    | exp '/' exp
    | '-' exp
    | '(' exp ')'
single_value : INTEGER
             | DOUBLE
             | CHAR
             | STRING
ag_ruleset : ag_rule
           | ag_ruleset ag_rule
ag_rule : ag_ruleid IF premise THEN conclusion property comment
ag_ruleid : GR
          | AR
```

Fig A.1 (continued)

functions (see Fig 2.3 and Fig 2.5 in [13]).

Table A.1: Symbols used in defining MOSAA grammars.

Symbol	Meaning
:	is defined to be
|	alternatively
lowercase words (e.g. `premise`, `rulelist`)	nonterminal
uppercase words (e.g. `CR`, `IDENTIFIER`)	both are terminal
'single_char' (e.g. `'='`, `'%'`, `'+'`)	
*	The preceding syntactic unit can be repeated zero or more times
+	The preceding syntactic unit can be repeated one or more times
{}	The enclosed syntactic units are grouped as a single syntactic unit
[]	The enclosed syntactic unit is optional, may occur zero or one time

Appendix B

Assignments for the spectrum of $CH_3^{18}OH$ in the 900-1100 cm^{-1} region.

B.1 Some of the previously assigned series in spreadsheet format.

O-18 Methanol K=0 A n=0 (010) A															
											Calculated	Observed			
	R Branch					P Branch					R-P Diff	R-P Diff	R-P Diff	Δ1(R-P)	Δ2(R-P)
J	R(J)	Δ1	Δ2	Int.	J	P(J)	Δ1	Δ2	Int.	J	R(J)-P(J+2)	R(J)-P(J+2)	Obs-Calc		
	1007.948070					1007.950169									
0	1009.478034	1.512668		0.7530	0					0	4.63954	4.639156	-0.00038	0.00044	
1	1010.990702	1.495372	-0.017296	0.6197	1	1006.402789	-1.563911		0.5529	1	7.73221	7.732266	0.00006	-0.00010	-0.00054
2	1012.486074	1.478293	-0.017079	0.4738	2	1004.838878	-1.580442	-0.016531	0.5246	2	10.82436	10.824317	-0.00004	0.00011	0.00021
3	1013.964367	1.461013	-0.017280	0.3872	3	1003.258436	-1.596679	-0.016237	0.4750	3	13.91576	13.915828	0.00007	0.00013	0.00002
4	1015.425380	1.443217	-0.017796	0.3004	4	1001.661757	-1.613218	-0.016539	0.3958	4	17.00622	17.006420	0.00020	-0.00018	-0.00031
5	1016.868597	1.425843	-0.017374	0.2677	5	1000.048539	-1.629579	-0.016361	0.3218	5	20.09552	20.095538	0.00002	0.00007	0.00025
6	1018.294440	1.408141	-0.017702	0.2371	6	998.418960	-1.645901	-0.016322	0.2896	6	23.18345	23.183534	0.00008	-0.00005	-0.00011
7	1019.702581	1.390439	-0.017702	0.2251	7	996.773059	-1.662153	-0.016252	0.2562	7	26.26980	26.269837	0.00004	0.00010	0.00015
8	1021.093020	1.372526	-0.017913	0.2041	8	995.110906	-1.678162	-0.016009	0.2202	8	29.35435	29.354486	0.00014	0.00007	-0.00003
9	1022.465546	1.354544	-0.017982	0.1902	9	993.432744	-1.694210	-0.016048	0.1970	9	32.43690	32.437108	0.00021	0.00009	0.00001
10	1023.820090	1.336475	-0.018069	0.1865	10	991.738534	-1.710096	-0.015886	0.1994	10	35.51723	35.517524	0.00029	0.00013	0.00005
11	1025.156565	1.318298	-0.018177	0.1916	11	990.028438	-1.725872	-0.015776	0.1893	11	38.59514	38.595568	0.00043	0.00019	0.00006
12	1026.474863	1.300135	-0.018163	0.1736	12	988.302566	-1.741569	-0.015697	0.1951	12	41.67042	41.671040	0.00062	0.00038	0.00018
13	1027.774998	1.281724	-0.018411	0.1818	13	986.560997	-1.757174	-0.015605	0.2020	13	44.74284	44.743836	0.00100	0.00045	0.00007
14	1029.056722	1.263382	-0.018342	0.2094	14	984.803823	-1.772661	-0.015487	0.2082	14	47.81221	47.813654	0.00144	0.00062	0.00017
15	1030.320104	1.244706	-0.018676	0.2059	15	983.031162	-1.788094	-0.015433	0.2208	15	50.87831	50.880375	0.00206	0.00085	0.00023
16	1031.564810	1.226364	-0.018342	0.2166	16	981.243068	-1.803339	-0.015245	0.2366	16	53.94093	53.943845	0.00292	0.00130	0.00045
17	1032.791174	1.207633	-0.018731	0.2497	17	979.439729	-1.818764	-0.015425	0.0814	17	56.99986	57.004074	0.00421	0.00144	0.00014
18	1033.998807	1.188964	-0.018669	0.2836	18	977.620965	-1.833865	-0.015101	0.2915	18	60.05489	60.060545	0.00565	0.00203	0.00056
19	1035.187771	1.170591	-0.018373	0.3123	19	975.787100	-1.848838	-0.014973	0.2184G*	19	63.10580	63.113480	0.00768	0.00292	0.00089
20	1036.358362	1.151221	-0.019370	0.3206	20	973.938262	-1.863971	-0.015133	0.3610	20	66.15239	66.162990	0.01060	0.00303	0.00011
21	1037.509583	1.132707	-0.018514	0.3943	21	972.074291	-1.878919	-0.014948	0.3889	21	69.19445	69.208083	0.01363	0.00411	0.00108
22	1038.642290	1.113961	-0.018746	0.4552	22	970.195372	-1.893872	-0.014953	0.4276	22	72.23176	72.249506	0.01775	0.00519	0.00106
23	1039.756251	1.095120	-0.018641	0.4950	23	968.301500	-1.908716	-0.014844	0.4181G*	23	75.26411	75.287045	0.02294	0.00634	0.00115
24	1040.851371	1.076342	-0.018778	0.5373	24	966.392784	-1.923578	-0.014862	0.5247	24	78.29130	78.320571	0.02927	0.00769	0.00136
25	1041.927713	1.057517	-0.018825	0.5564	25	964.469206	-1.938406	-0.014828	0.5637	25	81.31311	81.350074	0.03696	0.00934	0.00164
26	1042.985230	1.038646	-0.018871	0.6255	26	962.530800	-1.953161	-0.014755	0.3908G*	26	84.32933	84.375630	0.04630	0.01107	0.00173
27	1044.023876	1.020085	-0.018561	0.6676	27	960.577639	-1.968039	-0.014878	0.6586	27	87.33975	87.397117	0.05737	0.01334	0.00228
28	1045.043961	1.001401	-0.018684	0.7067	28	958.609600	-1.982841	-0.014802	0.6823G*	28	90.34416	90.414869	0.07071	0.01571	0.00236
29	1046.045362	0.982436	-0.018965	0.7450	29	956.626759	-1.997667	-0.014826	0.7563	29	93.34235	93.428765	0.08642	0.01808	0.00238
30	1047.027798	0.963892	-0.018544	0.7896	30	954.629092	-2.012495	-0.014828	0.7819	30	96.33410	96.438598	0.10450	0.02098	0.00290
31	1047.991690	0.945035	-0.018857	0.7864	31	952.616597	-2.027397	-0.014902	0.8200	31	99.31921	99.444690	0.12548	0.02400	0.00302
32	1048.936725	0.927162	-0.017873	0.8454	32	950.589200	-2.042200	-0.014803	0.8376G*	32	102.29747	102.446947	0.14948	0.02820	0.00420
33	1049.863887	0.908072	-0.019090	0.8798	33	948.547000	-2.057222	-0.015022	0.8655G*	33	105.26866	105.446335	0.17767	0.03112	0.00292
34	1050.771959	0.889325	-0.018747	0.8391	34	946.489778	-2.072226	-0.015004	0.8919	34	108.23258	108.441375	0.20879	0.03522	0.00410
35	1051.661284	0.871031	-0.018294	0.8771	35	944.417552	-2.086968	-0.014742	0.9165	35	111.18901	111.433023	0.24401	0.03951	0.00429
36	1052.532315	0.852985	-0.018046	0.9337	36	942.330584	-2.102323	-0.015355	0.9155	36	114.13774	114.421260	0.28352	0.04467	0.00517
37	1053.385300	0.834300	-0.018685	0.9243	37	940.228261	-2.117206	-0.014883	0.9462	37	117.07856	117.406755	0.32819		
38	1054.219600	0.815523	-0.018777	.9542G*B	38	938.111055	-2.132510	-0.015304	0.9534			#########			
39	1055.035123	0.796480	-0.019043	0.9473	39	935.978545	-935.978545	-933.846035	0.9620			#########			
40	1055.831603	0.779385	-0.017095	0.9492								#########			
41	1056.610988	0.758658	-0.020727	0.9650								#########			
42	1057.369646	##########	-1056.128304	0.9718								#########			

O-18 Methanol K=1 E2 n=0 (011) E2

	R Branch						P Branch						Q Branch		
J	R(J)	Δ1	Δ2	Int.	C	J	P(J)	Δ1	Δ2	Int.	C	J	Q(J)	Δ1	Δ2
	1008.256399						1008.259340						1008.256973		
1	1011.299052	1.495231		0.6827		1						1	1008.240035	-0.033876	
2	1012.794283	1.477834	-0.017397	0.5376		2	1005.147454	-1.580333		0.6398		2	1008.206159	-0.050797	-0.016921
3	1014.272117	1.460279	-0.017555	0.4220		3	1003.567121	-1.596593	-0.016260	0.5266		3	1008.155362	-0.066925	-0.016128
4	1015.732396	1.442773	-0.017506	0.3491		4	1001.970528	-1.613008	-0.016415	0.4314		4	1008.088437	##########	-1008.021512
5	1017.175169	1.424587	-0.018186	0.2665		5	1000.357520	-1.629337	-0.016329	0.3568		5		0.000000	1008.088437
6	1018.599756	1.407003	-0.017584	0.2171		6	998.728183	-1.645488	-0.016151	0.2939		6		0.000000	0.000000
7	1020.006759	1.388426	-0.018577	0.1930		7	997.082695	-1.661567	-0.016079	0.2580		7		0.000000	0.000000
8	1021.395185	1.370562	-0.017864	0.2001		8	995.421128	-1.677406	-0.015839	0.2457		8		0.000000	0.000000
9	1022.765747	1.352071	-0.018491	0.1945		9	993.743722	-1.693283	-0.015877	0.2184		9		0.000000	0.000000
10	1024.117818	1.333582	-0.018489	0.1930		10	992.050439	-1.708957	-0.015674	0.2101		10		0.000000	0.000000
11	1025.451400	1.314898	-0.018684	0.1999		11	990.341482	-1.724640	-0.015683	0.2037		11		0.000000	0.000000
12	1026.766298	1.296275	-0.018623	0.1729		12	988.616842	-1.739924	-0.015284	0.1968		12		0.000000	0.000000
13	1028.062573	1.277255	-0.019020	0.2029		13	986.876918	-1.754756	-0.014832	0.2087		13		0.000000	0.000000
14	1029.339828	1.258439	-0.018816	0.2066		14	985.122162	-1.771390	-0.016634	0.0642		14		0.000000	0.000000
15	1030.598267	1.239902	-0.018537	0.0877		15	983.350772	-1.785957	-0.014567	0.2265		15		0.000000	0.000000
16	1031.838169	1.221654	-0.018248	0.2299		16	981.564815	-1.801374	-0.015417	0.2538		16		0.000000	0.000000
17	1033.059823	1.200755	-0.020899	0.1603		17	979.763441	-1.815980	-0.014606	0.2091		17		0.000000	0.000000
18	1034.260578	1.182725	-0.018030	0.2985		18	977.947461	-1.831319	-0.015339	0.2990		18		0.000000	0.000000
19	1035.443303	1.164228	-0.018497	0.3359		19	976.116142	-1.846323	-0.015004	0.3188		19		0.000000	0.000000
20	1036.607531	1.144826	-0.019402	0.2256		20	974.269819	-1.860976	-0.014653	0.3574		20		0.000000	0.000000
21	1037.752357	1.125954	-0.018872	0.2011		21	972.408843	-1.876838	-0.015862	0.2914		21		0.000000	0.000000
22	1038.878311	1.107270	-0.018684	0.4573		22	970.532005	-1.891279	-0.014441	0.3415		22		0.000000	0.000000
23	1039.985581	1.089006	-0.018264	0.4549		23	968.640726	-1.906432	-0.015153	0.4773		23		0.000000	0.000000
24	1041.074587	1.070213	-0.018793	0.5457		24	966.734294	-1.921576	-0.015144	0.5308		24		0.000000	0.000000
25	1042.144800	1.051871	-0.018342	0.5527		25	964.812718	-1.936396	-0.014820	0.5622		25		0.000000	0.000000
26	1043.196671	1.033499	-0.018372	0.6270		26	962.876322	-1.951537	-0.015141	0.6246		26		0.000000	0.000000
27	1044.230170	1.015235	-0.018264	0.6838		27	960.924785	-1.966622	-0.015085	0.6697		27		0.000000	0.000000
28	1045.245405	0.997034	-0.018201	0.7222		28	958.958163	-1.981743	-0.015121	0.7220		28		0.000000	0.000000
29	1046.242439	0.979020	-0.018014	0.7598		29	956.976420	-1.996845	-0.015102	0.7596		29		0.000000	0.000000
30	1047.221459	0.960913	-0.018107	0.7939		30	954.979575	-2.011855	-0.015010	0.7857		30		0.000000	0.000000
31	1048.182372	0.943133	-0.017780	0.8084		31	952.967720	-2.027067	-0.015212	0.8142		31		0.000000	0.000000
32	1049.125505	0.925181	-0.017952	0.8481		32	950.940653	-2.042780	-0.015713	0.8459		32			
33	1050.050686	0.907386	-0.017795	0.8902		33	948.897873	-2.056598	-0.013818	0.8194					
34	1050.958072	0.889777	-0.017609	0.9028		34	946.841275	-2.072241	-0.015643	0.9055					
35	1051.847849	0.871794	-0.017983	0.9210		35	944.769034	-2.087160	-0.014919	0.9208					
36	1052.719643	0.854608	-0.017186	0.9311		36	942.681874	-2.102654	-0.015494	0.9220					
37	1053.574251	##########	-1054.428859	0.9493		37	940.579220	-2.116715	-0.014061	0.9409					
						38	938.462505	-2.131761	-0.015046	0.9512					
						39	936.330744	-936.330744	-934.198983	0.9642					

		Calculated	Observed						Ground State Vco=0		Excited State Vco=1		
		R-P Diff	R-P Diff	R-P Diff	Δ1(R-P)	Δ2(R-P)	R-P Diff	a-Type Freq	R(J) a-Type Frequencies		R(J) a-Type Frequencies		
Int.	J	R(J)-P(J+2)	R(J)-P(J+2)	Obs-Calc			MW Obsvns	Microwave	R(J)-Q(J+1)	Q(J)-P(J+1)	R(J)-Q(J)	Q(J+1)-P(J+1)	J
0.6455	1	7.73193	7.731931	0.00000	0.00002		7.731946	92723.32	3.092893	3.092581	3.059017	3.058705	1
0.7974	2	10.82373	10.823755	0.00003	0.00001	-0.00001	10.823758	139074.60	4.638921	4.639038	4.588124	4.588241	2
0.8458	3	13.91456	13.914597	0.00004	0.00003	0.00001		185413.51	6.183680	6.184834	6.116755	6.117909	3
0.5613	4	17.00415	17.004213	0.00006	0.00021	0.00018		x	##########	7.730917	7.643959	-1000.357520	4
	5	20.09220	20.092474	0.00027	-0.00011	-0.00032			##########	-998.728183	##########	-998.728183	5
	6	23.17846	23.178628	0.00017	0.00024	0.00034			##########	-997.082695	##########	-997.082695	6
	7	26.26263	26.263037	0.00041	-0.00011	-0.00035			##########	-995.421128	##########	-995.421128	7
	8	29.34445	29.344746	0.00030	0.00033	0.00044			##########	-993.743722	##########	-993.743722	8
	9	32.42364	32.424265	0.00062	0.00044	0.00011			##########	-992.050439	##########	-992.050439	9
	10	35.49991	35.500976	0.00107	0.00043	-0.00001			##########	-990.341482	##########	-990.341482	10
	11	38.57299	38.574482	0.00149	0.00003	-0.00039			##########	-988.616842	##########	-988.616842	11
	12	41.64261	41.644136	0.00153	0.00179	0.00176			##########	-986.876918	##########	-986.876918	12
	13	44.70848	44.711801	0.00332	0.00136	-0.00043			##########	-985.122162	##########	-985.122162	13
	14	47.77033	47.775013	0.00468	0.00226	0.00090			##########	-983.350772	##########	-983.350772	14
	15	50.82788	50.834826	0.00695	0.00290	0.00064			##########	-981.564815	##########	-981.564815	15
	16	53.88086	53.890708	0.00985	0.00485	0.00195			##########	-979.763441	##########	-979.763441	16
	17	56.92898	56.943681	0.01470	0.00408	-0.00078			##########	-977.947461	##########	-977.947461	17
	18	59.97198	59.990759	0.01878	0.00612	0.00204			##########	-976.116142	##########	-976.116142	18
	19	63.00956	63.034460	0.02490	0.00916	0.00304			##########	-974.269819	##########	-974.269819	19
	20	66.04147	66.075526	0.03406	0.01018	0.00102			##########	-972.408843	##########	-972.408843	20
	21	69.06740	69.111631	0.04423	0.01269	0.00251			##########	-970.532005	##########	-970.532005	21
	22	72.08710	72.144017	0.05692	0.01566	0.00297			##########	-968.640726	##########	-968.640726	22
	23	75.10029	75.172863	0.07257	0.01902	0.00337			##########	-966.734294	##########	-966.734294	23
	24	78.10667	78.198265	0.09160	0.02243	0.00341			##########	-964.812718	##########	-964.812718	24
	25	81.10599	81.220015	0.11402	0.02652	0.00409			##########	-962.876322	##########	-962.876322	25
	26	84.09796	84.238508	0.14055	0.03090	0.00438			##########	-960.924785	##########	-960.924785	26
	27	87.08230	87.253750	0.17145	0.03564	0.00474			##########	-958.958163	##########	-958.958163	27
	28	90.05874	90.265830	0.20709	0.04063	0.00499			##########	-956.976420	##########	-956.976420	28
	29	93.02700	93.274719	0.24772	0.04630	0.00567			##########	-954.979575	##########	-954.979575	29
	30	95.98679	96.280806	0.29402	0.05262	0.00633							30
	31	98.93786	99.284499	0.34664	0.05768	0.00506							31
	32	101.87991	102.284230	0.40432	0.06466	0.00698							32
	33	104.81267	105.281652	0.46898	0.07136	0.00669							33
	34	107.73586	108.276198	0.54034	0.07908	0.00773							34
	35	110.64921	111.268629	0.61942	0.08528	0.00620							35
	36	113.55244	114.257138	0.70470	0.09355	0.00827							36
	37	116.44526	117.243507	0.79825									
	38	119.32741											

O-18 Methanol K=3 A+ n=0 (013+)															
	R Branch	[Series K]					P Branch						Q Branch		
J	R(J)	Δ1	Δ2	Int.	C	J	P(J)	Δ1	Δ2	Int.	C	J	Q(J) + <- -	Δ1	Δ2
	1008.174105						1008.179991						1008.177945		
3	1014.194415	1.461660		0.4763		3						3	1008.076436	-0.067673	
4	1015.656075	1.444293	-0.017367	0.2702		4	1001.890737	-1.613936		0.4981		4	1008.008763	-0.084400	-0.016727
5	1017.100368	1.427395	-0.016898	0.1926		5	1000.276801	-1.630585	-0.016649	0.2988		5	1007.924363	-0.102157	-0.017757
6	1018.527763	1.410106	-0.017289	0.1546		6	998.646216	-1.647492	-0.016907	0.1903	•	6	1007.822206	-0.118931	-0.016774
7	1019.937869	1.392958	-0.017148	0.1143		7	996.998724	-1.664235	-0.016743	0.1306	•	7	1007.703275	-0.136141	-0.017210
8	1021.330827	1.375677	-0.017281	0.0879	•	8	995.334489	-1.681141	-0.016906	0.0994	•	8	1007.567134	-0.151567	-0.015426
9	1022.706504	1.358770	-0.016907	0.0860		9	993.653348	-1.696956	-0.015815	0.0604	•	9	1007.415567	-0.169151	-0.017584
10	1024.065274	1.340764	-0.018006	0.0450	•	10	991.956392	-1.716451	-0.019495	0.0464	•	10	1007.246416	-0.186214	-0.017063
11	1025.406038	1.324232	-0.016532	0.0745		11	990.239941	-1.730293	-0.013842	0.0277	•	11	1007.060202	-0.205951	-0.019737
12	1026.730270	1.305228	-0.019004	0.0770		12	988.509648	-1.747902	-0.017609	0.0450	•	12	1006.854251	-0.220362	-0.014411
13	1028.035498	1.286964	-0.018264	0.0531		13	986.761746	-1.763997	-0.016095	0.0381	•	13	1006.633889	-0.242065	-0.021703
14	1029.322462	1.271516	-0.015448	0.1078		14	984.997749	-1.780560	-0.016563	0.0565	•	14	1006.391824	-0.262839	-0.020774
15	1030.593978	1.253050	-0.018466	0.2690		15	983.217189	-1.797288	-0.016728	0.0582	•	15	1006.128985	##########	-1005.866146
16	1031.847028	1.235347	-0.017703	0.3012		16	981.419901	-1.813758	-0.016470	0.0829		16		0.000000	1006.128985
17	1033.082375	1.216866	-0.018481	0.3072		17	979.606143	-1.830243	-0.016485	0.1334		17		0.000000	0.000000
18	1034.299241	1.199710	-0.017156	0.3077		18	977.775900	-1.846700	-0.016457	0.1372*G		18		0.000000	0.000000
19	1035.498951	1.181447	-0.018263	0.3910		19	975.929200	-1.863104	-0.016404	0.2907*G		19		0.000000	0.000000
20	1036.680398	1.163385	-0.018062	0.4328		20	974.066096	-1.879596	-0.016492	0.3584		20		0.000000	0.000000
21	1037.843783	1.145201	-0.018184	0.4791		21	972.186500	-1.895881	-0.016285	0.2725*G		21		0.000000	0.000000
22	1038.988984	1.127670	-0.017531	0.4744		22	970.290619	-1.912046	-0.016165	0.4622		22		0.000000	0.000000
23	1040.116654	1.109172	-0.018498	0.3097		23	968.378573	-1.928056	-0.016010	0.5012		23		0.000000	0.000000
24	1041.225826	1.093081	-0.016091	0.6044		24	966.450517	-1.944370	-0.016314	0.4899		24		0.000000	0.000000
25	1042.318907	1.088082	-0.004999	0.6555		25	964.506147	-1.960189	-0.015819	0.4667		25		0.000000	0.000000
26	1043.406989	1.012834	-0.075248	0.7111		26	962.545958	-1.973633	-0.013444	0.3594		26		0.000000	0.000000
27	1044.419823	1.042263	0.029429	0.7091		27	960.572325	-1.976327	-0.002694	0.7209		27		0.000000	0.000000
28	1045.462086	1.017372	-0.024891	0.5350		28	958.595998	-2.046726	-0.070399	0.7983		28		0.000000	0.000000
29	1046.479458	0.996083	-0.021289	0.6732		29	956.549272	-2.018804	0.027922	0.6952		29		0.000000	0.000000
30	1047.475541	0.977663	-0.018420	0.7816		30	954.530468	-2.039540	-0.020736	0.7823		30		0.000000	0.000000
31	1048.453204	0.958152	-0.019511	0.8536		31	952.490928	-2.058485	-0.018945	0.7670		31		0.000000	0.000000
32	1049.411356	0.939203	-0.018949	0.9199		32	950.432443	-2.075139	-0.016654	0.8194		32			
33	1050.350559	0.919629	-0.019574	0.8947		33	948.357304	-2.093390	-0.018251	0.8693	•				
34	1051.270188	0.899774	-0.019855	0.9100		34	946.263914	-2.108554	-0.015164	0.8755	•				
35	1052.169962	0.881667	-0.018107	0.8863		35	944.155360	-2.126692	-0.018138	0.8895	•				
36	1053.051629	0.861891	-0.019776	0.8664	•	36	942.028668	-2.139677	-0.012985	0.9367	•				
37	1053.913520	0.844938	-0.016953	0.9162	•	37	939.888991	-939.888991	-937.749314	0.9248					
38	1054.758458	0.820342	-0.024596	0.8991	•										
39	1055.578800	0.802359	-0.017983	0.9546											
40	1056.381159	0.784517	-0.017842	0.9631											
41	1057.165676	##########	-1057.950193	0.8866											

		Calculated	Observed				Ground State Vco=0		Excited State Vco=1			Gd State
		R-P Diff	R-P Diff	R-P Diff	Δ1(R-P)	Δ2(R-P)	R(J) a-Type Frequencies		R(J) a-Type Frequencies			Splitting
Int.	J	R(J)-P(J+2)	R(J)-P(J+2)	Obs-Calc			R(J)-Q(J+1)	Q(J)-P(J+1)	R(J)-Q(J)	Q(J+1)-P(J+1)	J	
0.1393	3	13.91743	13.917614	0.00018	-0.00001		6.185652	6.185699	6.117979	6.118026	3	0.000000
0.2181	4	17.00969	17.009859	0.00017	-0.00016	-0.00015	7.731712	7.731962	7.647312	7.647562	4	0.000003
0.0318	5	20.10164	20.101644	0.00001	0.00006	0.00022	9.278162	9.278147	9.176005	9.175990	5	0.000013
0.1519	6	23.19321	23.193274	0.00007	0.00011	0.00005	10.824488	10.823482	10.705557	10.704551	6	0.000040
0.2692	7	26.28435	26.284521	0.00017	-0.00072	-0.00082	12.370735	12.368786	12.234594	12.232645	7	0.000101
0.4218	8	29.37498	29.374435	-0.00054	0.00208	0.00279	13.915260	13.913786	13.763693	13.762219	8	0.000223
0.5493	9	32.46503	32.466563	0.00153	-0.00034	-0.00241	15.460088	15.459175	15.290937	15.290024	9	0.000445
0.5948	10	35.55443	35.555626	0.00119	0.00001	0.00035	17.005072	17.006475	16.818858	16.820261	10	0.000827
0.5061	11	38.64308	38.644292	0.00121	0.00040	0.00039	18.551787	18.550554	18.345836	18.344603	11	0.001445
0.7550	12	41.73091	41.732521	0.00161	-0.00112	-0.00152	20.096381	20.092505	19.876019	19.872143	12	0.002404
0.5020	13	44.81782	44.818309	0.00049	-0.00166	-0.00054	21.643674	21.636140	21.401609	21.394075	13	0.003839
0.6966	14	47.90373	47.902561	-0.00117	0.00050	0.00216	23.193477	23.174635	22.930638	22.911796	14	0.005921
0.6295	15	50.98851	50.987835	-0.00067	-0.00027	-0.00077	##########	24.709084	24.464993	-981.419901	15	0.008863
	16	54.07207	54.071128	-0.00094	-0.00018	0.00009	##########	-979.606143	##########	-979.606143	16	0.012900
	17	57.15430	57.153175	-0.00112	-0.00042	-0.00024	##########	-977.775900	##########	-977.775900	17	0.018370
	18	60.23469	60.233145	-0.00155	0.00038	0.00081	##########	-975.929200	##########	-975.929200	18	0.025600
	19	63.31361	63.312451	-0.00116	-0.00003	-0.00042	##########	-974.066096	##########	-974.066096	19	0.035035
	20	66.39097	66.389779	-0.00119	-0.00061	-0.00058	##########	-972.186500	##########	-972.186500	20	0.047920
	21	69.46702	69.465210	-0.00180	-0.00014	0.00047	##########	-970.290619	##########	-970.290619	21	0.063850
	22	72.54042	72.538467	-0.00195	0.00134	0.00148	##########	-968.378573	##########	-968.378573	22	0.084134
	23	75.61112	75.610507	-0.00061	0.00050	-0.00083	##########	-966.450517	##########	-966.450517	23	0.107780
	24	78.67998	78.679868	-0.00011	0.00076	0.00026	##########	-964.506147	##########	-964.506147	24	0.138640
	25	81.74593	81.746582	0.00065	0.00039	-0.00037	##########	-962.545958	##########	-962.545958	25	0.175742
	26	84.80995	84.810991	0.00104	-0.00181	-0.00220	##########	-960.572325	##########	-960.572325	26	0.221087
	27	87.87131	87.870551	-0.00076	0.00378	0.00559	##########	-958.595998	##########	-958.595998	27	0.275739
	28	90.92860	90.931618	0.00302	0.00162	-0.00217	##########	-956.549272	##########	-956.549272	28	0.339652
	29	93.98390	93.988530	0.00463	0.00243	0.00081	##########	-954.530468	##########	-954.530468	29	0.415210
	30	97.03603	97.043098	0.00706	0.00318	0.00075	##########	-952.490928	##########	-952.490928	30	0.505134
	31	100.08566	100.095900	0.01024	0.00426	0.00108	##########	-950.432443	##########	-950.432443	31	0.607479
	32	103.13294	103.147442	0.01450	0.00406	-0.00020	##########	-948.357304	##########	-948.357304	32	0.727126
	33	106.17664	106.195199	0.01856	0.00561	0.00155					33	0.861042
	34	109.21734	109.241520	0.02418	0.00307	-0.00254					34	1.013328
	35	112.25372	112.280971	0.02725	936.82542	936.82235					35	1.183451
	36	116.19896	##########	936.85267	-2.29885	-939.12427					36	1.374205
		119.35970	##########	934.55382	-1.41322	0.88563						1.587606
		121.61786	##########	933.14060	122.43820	123.85142						
			##########	1055.57880	-1055.57880	-1178.01700						
				0.00000								

O-18 Methanol K=3 A- n=0 (013-)

	R Branch	[Series H]					P Branch	[Series H]					Q Branch		
J	R(J)	Δ1	Δ2	Int.	C	J	P(J)	Δ1	Δ2	Int.	C	J	Q(J)	Δ1	Δ2
	1008.174105						1008.179991						1008.177945		
3	1014.194415	1.461660		0.4763		3						3	1008.076436	-0.067673	
4	1015.656075	1.444293	-0.017367	0.2702		4	1001.890737	-1.613936		0.4981		4	1008.008763	-0.084400	-0.016727
5	1017.100368	1.427395	-0.016898	0.1926		5	1000.276801	-1.630585	-0.016649	0.2988		5	1007.924363	-0.102157	-0.017757
6	1018.527763	1.410106	-0.017289	0.1546		6	998.646216	-1.647492	-0.016907	0.1903	*	6	1007.822206	-0.118931	-0.016774
7	1019.937869	1.392958	-0.017148	0.1143		7	996.998724	-1.664235	-0.016743	0.1306	*	7	1007.703275	-0.136141	-0.017210
8	1021.330827	1.375677	-0.017281	0.0879	*	8	995.334489	-1.681141	-0.016906	0.0994	*	8	1007.567134	-0.151567	-0.015426
9	1022.706504	1.358770	-0.016907	0.0860		9	993.653348	-1.696956	-0.015815	0.0604	*	9	1007.415567	-0.169151	-0.017584
10	1024.065274	1.340764	-0.018006	0.0450	*	10	991.956392	-1.716451	-0.019495	0.0464	*	10	1007.246416	-0.186214	-0.017063
11	1025.406038	1.324232	-0.016532	0.0745		11	990.239941	-1.730293	-0.013842	0.0277	*	11	1007.060202	-0.201825	-0.015611
12	1026.730270	1.305228	-0.019004	0.0770		12	988.509648	-1.747902	-0.017609	0.0450	*	12	1006.858377	-0.218686	-0.016861
13	1028.035498	1.290403	-0.014825	0.0531		13	986.761746	-1.763997	-0.016095	0.0381	*	13	1006.639691	-0.236902	-0.018216
14	1029.325901	1.272366	-0.018037	0.2587		14	984.997749	-1.783064	-0.019067	0.0565	*	14	1006.402789	-0.255119	-0.018217
15	1030.598267	1.254157	-0.018209	0.0877	*	15	983.214685	-1.798910	-0.015846	0.1966	*	15	1006.147670	##########	-1005.892551
16	1031.852424	1.236658	-0.017499	0.2339		16	981.415775	-1.815894	-0.016984	0.2889		16		0.000000	1006.147670
17	1033.089082	1.219268	-0.017390	0.3129	*	17	979.599881	-1.832419	-0.016525	0.2997		17		0.000000	0.000000
18	1034.308350	1.201909	-0.017359	0.3631		18	977.767462	-1.847820	-0.015401	0.1019	*	18		0.000000	0.000000
19	1035.510259	1.184347	-0.017562	0.3997		19	975.919642	-1.866965	-0.019145	0.1701	*	19		0.000000	0.000000
20	1036.694606	1.166895	-0.017452	0.4161		20	974.052677	-1.884409	-0.017444	0.3770		20		0.000000	0.000000
21	1037.861501	1.149302	-0.017593	0.4592		21	972.168268	-1.899655	-0.015246	0.2980	*	21		0.000000	0.000000
22	1039.010803	1.131866	-0.017436	0.4796		22	970.268613	-1.917591	-0.017936	0.4965		22		0.000000	0.000000
23	1040.142669	1.114194	-0.017672	0.5080		23	968.351022	-1.934833	-0.017242	0.5436		23		0.000000	0.000000
24	1041.256863	1.096618	-0.017576	0.5631		24	966.416189	-1.951989	-0.017156	0.5827		24		0.000000	0.000000
25	1042.353481	1.079055	-0.017563	0.6474		25	964.464200	-1.969652	-0.017663	0.6055		25		0.000000	0.000000
26	1043.432536	1.061541	-0.017514	0.6877		26	962.494548	-1.987646	-0.017994	0.6684		26		0.000000	0.000000
27	1044.494077	1.043948	-0.017593	0.7290		27	960.506902	-2.003922	-0.016276	0.6427	*	27		0.000000	0.000000
28	1045.538025	1.026138	-0.017810	0.7553		28	958.502980	-2.022180	-0.018258	0.7462		28		0.000000	0.000000
29	1046.564163	1.009058	-0.017080	0.6944	*	29	956.480800	-2.039875	-0.017695	0.7856		29		0.000000	0.000000
30	1047.573221	0.991155	-0.017903	0.8174		30	954.440925	-2.057561	-0.017686	0.8132		30		0.000000	0.000000
31	1048.564376	0.973467	-0.017688	0.8635		31	952.383364	-2.075233	-0.017672	0.8563		31		0.000000	0.000000
32	1049.537843	0.956063	-0.017404	0.8562		32	950.308131	-2.093218	-0.017985	0.8737		32			
33	1050.493906	0.940094	-0.015969	0.8994		33	948.214913	-2.110714	-0.017496	0.8972					
34	1051.434000	0.922699	-0.017395			34	946.104199	-2.127901	-0.017187	0.9054					
35	1052.356699	##########	-1053.279398	0.9428		35	943.976298	-2.144695	-0.016794	0.9222					
36		0.000000	1052.356699			36	941.831603	-2.160030	-0.015335	0.8999	*				
37		0.000000	0.000000			37	939.671573	-939.671573	-937.511543	0.9621	#				

		Calculated	Observed				Ground State Vco=0		Excited State Vco=1			Gd State
		R-P Diff	R-P Diff	R-P Diff	Δ1(R-P)	Δ2(R-P)	R(J) a-Type Frequencies		R(J) a-Type Frequencies			Splitting
Int.	J	R(J)-P(J+2)	R(J)-P(J+2)	Obs-Calc			R(J)-Q(J+1)	Q(J)-P(J+1)	R(J)-Q(J)	Q(J+1)-P(J+1)	J	
0.1393	3	13.91745	13.917614	0.00017	-0.00004		6.185652	6.185699	6.117979	6.118026	3	0.000000
0.2181	4	17.00973	17.009859	0.00013	-0.00021	-0.00017	7.731712	7.731962	7.647312	7.647562	4	0.000003
0.0318	5	20.10172	20.101644	-0.00008	-0.00004	0.00017	9.278162	9.278147	9.176005	9.175990	5	0.000013
0.1519	6	23.19339	23.193274	-0.00012	-0.00005	-0.00002	10.824488	10.823482	10.705557	10.704551	6	0.000040
0.2692	7	26.28469	26.284521	-0.00017	-0.00098	-0.00092	12.370735	12.368786	12.234594	12.232645	7	0.000101
0.4218	8	29.37558	29.374435	-0.00115	0.00168	0.00266	13.915260	13.913786	13.763693	13.762219	8	0.000223
0.5493	9	32.46603	32.466563	0.00053	-0.00092	-0.00260	15.460088	15.459175	15.290937	15.290024	9	0.000445
0.5948	10	35.55601	35.555626	-0.00038	-0.00080	0.00011	17.005072	17.006475	16.818858	16.820261	10	0.000827
0.5061	11	38.64548	38.644292	-0.00118	-0.00072	0.00008	18.547661	18.550554	18.345836	18.348729	11	0.001445
0.7856	12	41.73443	41.732521	-0.00191	-0.00012	0.00060	20.090579	20.096631	19.871893	19.877945	12	0.002404
0.4732	13	44.82284	44.820813	-0.00203	0.00145	0.00157	21.632709	21.641942	21.395807	21.405040	13	0.003839
0.5529	14	47.91071	47.910126	-0.00058	0.00096	-0.00049	23.178231	23.188104	22.923112	22.932985	14	0.005921
0.9402	15	50.99801	50.998386	0.00037	-0.00018	-0.00114	##########	24.731895	24.450597	-981.415775	15	0.008863
	16	54.08477	54.084962	0.00019	-0.00171	-0.00153	##########	-979.599881	##########	-979.599881	16	0.012900
	17	57.17096	57.169440	-0.00152	0.00019	0.00190	##########	-977.767462	##########	-977.767462	17	0.018370
	18	60.25701	60.255673	-0.00134	0.00090	0.00071	##########	-975.919642	##########	-975.919642	18	0.025600
	19	63.34243	63.341991	-0.00044	-0.00076	-0.00166	##########	-974.052677	##########	-974.052677	19	0.035035
	20	66.42719	66.425993	-0.00119	0.00073	0.00149	##########	-972.168268	##########	-972.168268	20	0.047920
	21	69.51095	69.510479	-0.00047	0.00016	-0.00057	##########	-970.268613	##########	-970.268613	21	0.063850
	22	72.59492	72.594614	-0.00031	-0.00030	-0.00046	##########	-968.351022	##########	-968.351022	22	0.084134
	23	75.67908	75.678469	-0.00061	0.00050	0.00081	##########	-966.416189	##########	-966.416189	23	0.107780
	24	78.76242	78.762315	-0.00011	0.00076	0.00026	##########	-964.464200	##########	-964.464200	24	0.138640
	25	81.84593	81.846579	0.00065	0.00039	-0.00037	##########	-962.494548	##########	-962.494548	25	0.175742
	26	84.92851	84.929556	0.00104	0.00145	0.00106	##########	-960.506902	##########	-960.506902	26	0.221087
	27	88.01079	88.013277	0.00249	0.00053	-0.00092	##########	-958.502980	##########	-958.502980	27	0.275739
	28	91.09408	91.097100	0.00302	0.00162	0.00109	##########	-956.480800	##########	-956.480800	28	0.339652
	29	94.17616	94.180799	0.00463	0.00243	0.00081	##########	-954.440925	##########	-954.440925	29	0.415210
	30	97.25803	97.265090	0.00706	0.00318	0.00075	##########	-952.383364	##########	-952.383364	30	0.505134
	31	100.33922	100.349463	0.01024	0.00426	0.00108	##########	-950.308131	##########	-950.308131	31	0.607479
	32	103.41914	103.433644	0.01450	0.00406	-0.00020	##########	-948.214913	##########	-948.214913	32	0.727126
	33	106.49904	106.517608	0.01856	0.00562	0.00155					33	0.861042
	34	109.57822	109.602397	0.02418	0.00307	-0.00255					34	1.013328
	35	112.65788	112.685126	0.02725	-114.85201	-114.85508					35	1.183451
	36	114.82476	0.000000	-114.82476	-2.94734	111.90467					36	1.374205
		117.77210	0.000000	-117.77210	-3.84576	-0.89842						1.587606
		121.61786	0.000000	-121.61786	121.61786	125.46362						
			0.000000	0.00000	0.00000	-121.61786						
				0.00000								

O-18Methanol K=5 E1 n=0 (015)															
	R Branch	[Series N]					P Branch	[Series N]					Q Branch		
J	R(J)	Δ1	Δ2	Int.	C	J	P(J)	Δ1	Δ2	Int.	C	J	Q(J)	Δ1	Δ2
	1008.163480						1008.179565						1008.179755		
5	1017.095752	1.427168		0.5485	*	5						5	1007.924363	-0.102157	
6	1018.522920	1.409584	-0.017584	0.4119	*	6	998.646216	-1.647492		0.1903	*	6	1007.822206	-0.118931	-0.016774
7	1019.932504	1.391952	-0.017632	0.2722	*	7	996.998724	-1.664235	-0.016743	0.1306	*	7	1007.703275	-0.136141	-0.017210
8	1021.324456	1.374249	-0.017703	0.1698	*	8	995.334489	-1.681141	-0.016906	0.0994	*	8	1007.567134	-0.155162	-0.019021
9	1022.698705	1.357702	-0.016547	0.0723	*	9	993.653348	-1.696956	-0.015815	0.0604	*	9	1007.411972	-0.170469	-0.015307
10	1024.056407	1.336889	-0.020813	0.2884	*	10	991.956392	-1.716451	-0.019495	0.0464	*	10	1007.241503	-0.187196	-0.016727
11	1025.393296	1.317899	-0.018990	0.3838		11	990.239941	-1.730293	-0.013842	0.0277	*	11	1007.054307	-0.205936	-0.018740
12	1026.711195	1.305540	-0.012359	0.1485	*	12	988.509648	-1.747902	-0.017609	0.0451	*	12	1006.848371	-0.220671	-0.014735
13	1028.016735	1.287011	-0.018529	0.1087	*	13	986.761746	-1.763997	-0.016095	0.0381	*	13	1006.627700	-0.239704	-0.019033
14	1029.303746	1.267851	-0.019160	0.0904	*	14	984.997749	-1.780560	-0.016563	0.0565	*	14	1006.387996	-0.255996	-0.016292
15	1030.571597	1.249525	-0.018326	0.3490		15	983.217189	-1.797288	-0.016728	0.0582	*	15	1006.132000	-0.275024	-0.019028
16	1031.821122	1.232119	-0.017406	0.4185		16	981.419901	-1.813758	-0.016470	0.0829	*	16	1005.856976	-0.289307	-0.014283
17	1033.053241	1.214199	-0.017920	0.4369		17	979.606143	-1.829229	-0.015471	0.1334	*	17	1005.567669	-0.307070	-0.017763
18	1034.267440	1.196341	-0.017858	0.4716		18	977.776914	-1.851688	-0.022459	0.1372	*	18	1005.260599	-0.323783	-0.016713
19	1035.463781	1.178078	-0.018263	0.4779		19	975.925226	-1.862208	-0.010520	0.1701	*	19	1004.936816	-0.345040	-0.021257
20	1036.641859	1.160079	-0.017999	0.5449		20	974.063018	-1.879435	-0.017227	0.5074		20	1004.591776	-0.359295	-0.014255
21	1037.801938	1.142050	-0.018029	0.5556		21	972.183583	-1.897144	-0.017709	0.2725	*	21	1004.232481	-0.374931	-0.015636
22	1038.943988	1.123818	-0.018232	0.6228		22	970.286439	-1.912654	-0.015510	0.5887		22	1003.857550	-0.398793	-0.023862
23	1040.067806	1.105741	-0.018077	0.6476		23	968.373785	-1.929055	-0.016401	0.6294		23	1003.458757	-0.407270	-0.008477
24	1041.173547	1.087369	-0.018372	0.5930		24	966.444730	-1.945122	-0.016067	0.6287		24	1003.051487	##########	-1002.644217
25	1042.260916	1.067732	-0.019637	0.7125		25	964.499608	-1.961281	-0.016159	0.6940		25		0.000000	1003.051487
26	1043.328648	1.052277	-0.015455	0.4871	*	26	962.538327	-1.977571	-0.016290	0.7481		26		0.000000	0.000000
27	1044.380925	1.032235	-0.020042	0.7724		27	960.560756	-1.993631	-0.016060	0.7728		27		0.000000	0.000000
28	1045.413160	1.014003	-0.018232	0.8103		28	958.567125	-2.009727	-0.016096	0.8113		28		0.000000	0.000000
29	1046.427163	0.996036	-0.017967	0.8098		29	956.557398	-2.026930	-0.017203	0.8371		29		0.000000	0.000000
30	1047.423199	0.976681	-0.019355	0.7267	*	30	954.530468	-2.039540	-0.012610	0.7823	*	30		0.000000	0.000000
31	1048.399880	0.958558	-0.018123	0.8646		31	952.490928	-2.058485	-0.018945	0.7670	*	31		0.000000	0.000000
32	1049.358438	0.939046	-0.019512	0.8307	*	32	950.432443	-2.075139	-0.016654	0.8194	*	32			
33	1050.297484	0.923201	-0.015845	0.8607	*	33	948.357304	-2.088738	-0.013599	0.8693	*				
34	1051.220685	0.905623	-0.017578	0.9218		34	946.268566	-2.105423	-0.016685	0.9378					
35	1052.126308	##########	-1053.031931	0.9458		35	944.163143	-2.119070	-0.013647	0.9410					
36		0.000000	1052.126308			36	942.044073	-2.135208	-0.016138	0.9127	*				
37		0.000000	0.000000			37	939.908865	-939.908865	-937.773657	0.9536					
						38		0.000000	939.908865						

		Calculated	Observed				Ground State Vco=0		Excited State Vco=1		
		R-P Diff	R-P Diff	R-P Diff	Δ1(R-P)	Δ2(R-P)	R(J) a-Type Frequencies		R(J) a-Type Frequencies		
Int.	J	R(J)-P(J+2)	R(J)-P(J+2)	Obs-Calc			R(J)-Q(J+1)	Q(J)-P(J+1)	R(J)-Q(J)	Q(J+1)-P(J+1)	J
0.0318	5	20.09762	20.097028	-0.00059	0.00087		9.273546	9.278147	9.171389	9.175990	5
0.1519	6	23.18815	23.188431	0.00028	0.00080	-0.00007	10.819645	10.823482	10.700714	10.704551	6
0.2692	7	26.27807	26.279156	0.00109	-0.00032	-0.00113	12.365370	12.368786	12.229229	12.232645	7
0.4218	8	29.36730	29.368064	0.00076	0.00223	0.00255	13.912484	13.913786	13.757322	13.758624	8
0.2494	9	32.45577	32.458764	0.00299	0.00038	-0.00185	15.457202	15.455580	15.286733	15.285111	9
0.3812	10	35.54339	35.546759	0.00337	-0.00189	-0.00226	17.002100	17.001562	16.814904	16.814366	10
0.4201	11	38.63007	38.631550	0.00148	-0.00378	-0.00189	18.544925	18.544659	18.338989	18.338723	11
0.3442	12	41.71575	41.713446	-0.00230	0.00151	0.00529	20.083495	20.086625	19.862824	19.865954	12
	13	44.80034	44.799546	-0.00079	0.00088	-0.00063	21.628739	21.629951	21.389035	21.390247	13
0.7267	14	47.88376	47.883845	0.00009	-0.00055	-0.00143	23.171746	23.170807	22.915750	22.914811	14
	15	50.96592	50.965454	-0.00047	-0.00208	-0.00153	24.714621	24.712099	24.439597	24.437075	15
0.6173	16	54.04675	54.044208	-0.00254	0.00440	0.00647	26.253453	26.250833	25.964146	25.961526	16
0.3960	17	57.12616	57.128015	0.00186	-0.00152	-0.00592	27.792642	27.790755	27.485572	27.483685	17
0.6236	18	60.20409	60.204422	0.00033	-0.00056	0.00096	29.330624	29.335373	29.006841	29.011590	18
0.6788	19	63.28043	63.280198	-0.00023	0.00053	0.00110	30.872005	30.873798	30.526965	30.528758	19
0.8642	20	66.35512	66.355420	0.00030	-0.00022	-0.00075	32.409378	32.408193	32.050083	32.048898	20
0.8916	21	69.42807	69.428153	0.00008	-0.00003	0.00019	33.944388	33.946042	33.569457	33.571111	21
0.8947	22	72.49920	72.499258	0.00006	-0.00030	-0.00027	35.485231	35.483765	35.086438	35.084972	22
0.9461	23	75.56844	75.568198	-0.00024	-0.00023	0.00007	37.016319	37.014027	36.609049	36.606757	23
0.9441	24	78.63569	78.635220	-0.00047	-0.00025	-0.00002	##########	38.551879	38.122060	-964.499608	24
	25	81.70088	81.700160	-0.00072	-0.00169	-0.00144	##########	-962.538327	##########	-962.538327	25
	26	84.76393	84.761523	-0.00241	0.00117	0.00286	##########	-960.560756	##########	-960.560756	26
	27	87.82476	87.823527	-0.00123	0.00064	-0.00054	##########	-958.567125	##########	-958.567125	27
	28	90.88329	90.882692	-0.00060	-0.00260	-0.00323	##########	-956.557398	##########	-956.557398	28
	29	93.93943	93.936235	-0.00319	0.00084	0.00344	##########	-954.530468	##########	-954.530468	29
	30	96.99311	96.990756	-0.00235	0.00069	-0.00015					30
	31	100.04424	100.042576	-0.00166	-0.00121	-0.00190					31
	32	103.09275	103.089872	-0.00288	-0.00133	-0.00012					32
	33	106.13855	106.134341	-0.00421	-0.00074	0.00059					33
	34	109.18156	109.176612	-0.00495	0.00069	0.00143					34
	35	112.22170	112.217443	-0.00426	-115.25463	-115.25532					35
	36	115.25889	0.000000	-115.25889	-3.03416	112.22047					36
		118.29305		-118.29305							
		121.32410									

O-18 Methanol K=6 A n=0 (016)														
	R Branch	[Series L]					P Branch	[Series L]					Q Branch	
J	R(J)	Δ1	Δ2	Int.	C	J	P(J)	Δ1	Δ2	Int.	C	J	Q(J)	Δ1
	1008.196610						1008.214526						1008.188948	
6	1018.539320	1.408874		0.6539		6						6	1007.836133	-0.117605
7	1019.948194	1.391710	-0.017164	0.4710		7	997.017424	-1.664562		0.1944	*	7	1007.718528	-0.136110
8	1021.339904	1.373867	-0.017843	0.2955	*	8	995.352862	-1.680806	-0.016244	0.4966		8	1007.582418	-0.153094
9	1022.713771	1.356782	-0.017085	0.3282		9	993.672056	-1.697486	-0.016680	0.3914		9	1007.429324	-0.170220
10	1024.070553	1.338581	-0.018201	0.1859	*	10	991.974570	-1.714042	-0.016556	0.3355		10	1007.259104	-0.186939
11	1025.409134	1.321136	-0.017445	0.0938	*	11	990.260528	-1.730636	-0.016594	0.2988		11	1007.072165	-0.204813
12	1026.730270	1.305228	-0.015908	0.0770	*	12	988.529892	-1.747137	-0.016501	0.2753		12	1006.867352	-0.220884
13	1028.035498	1.286964	-0.018264	0.0531	*	13	986.782755	-1.764036	-0.016899	0.2463		13	1006.646468	-0.238330
14	1029.322462	1.268334	-0.018630	0.1078	*	14	985.018719	-1.779766	-0.015730	0.0938	*	14	1006.408138	-0.255298
15	1030.590796	1.251241	-0.017093	0.2368		15	983.238953	-1.796578	-0.016812	0.2742		15	1006.152840	-0.272337
16	1031.842037	1.233351	-0.017890	0.2644		16	981.442375	-1.812892	-0.016314	0.2752		16	1005.880503	-0.289587
17	1033.075388	1.215650	-0.017701	0.2837		17	979.629483	-1.829252	-0.016360	0.3030		17	1005.590916	-0.306221
18	1034.291038	1.197838	-0.017812	0.3195		18	977.800231	-1.845520	-0.016268	0.3244		18	1005.284695	-0.324063
19	1035.488876	1.180011	-0.017827	0.3479		19	975.954711	-1.861787	-0.016267	0.3441		19	1004.960632	-0.340197
20	1036.668887	1.162217	-0.017794	0.3302		20	974.092924	-1.877992	-0.016205	0.3794		20	1004.620435	-0.357128
21	1037.831104	1.143718	-0.018499	0.3091		21	972.214932	-1.894149	-0.016157	0.4171		21	1004.263307	-0.374821
22	1038.974822	1.126516	-0.017202	0.4128		22	970.320783	-1.910292	-0.016143	0.4468		22	1003.888486	-0.389756
23	1040.101338	1.108237	-0.018279	0.5116		23	968.410491	-1.926278	-0.015986	0.4909		23	1003.498730	-0.410709
24	1041.209575	1.090004	-0.018233	0.5473		24	966.484213	-1.942713	-0.016435	0.5074		24	1003.088021	-0.426796
25	1042.299579	1.071648	-0.018356	0.5789		25	964.541500	-1.957966	-0.015253	0.3455	*	25	1002.661225	-0.440748
26	1043.371227	1.055021	-0.016627	0.4211	*	26	962.583534	-1.974589	-0.016623	0.5294	*	26	1002.220477	-0.461608
27	1044.426248	1.035838	-0.019183	0.4550	*	27	960.608945	-1.989853	-0.015264	0.6570	*	27	1001.758869	-0.474249
28	1045.462086	1.017372	-0.018466	0.5351	*	28	958.619092	-2.005719	-0.015866	0.7143		28	1001.284620	-0.493113
29	1046.479458	1.000575	-0.016797	0.6732		29	956.613373	-2.021681	-0.015962	0.6210	*	29	1000.791507	-0.509942
30	1047.480033	0.981921	-0.018654	0.7962		30	954.591692	-2.037360	-0.015679	0.7844		30	1000.281565	-0.527604
31	1048.461954	0.964172	-0.017749	0.8298		31	952.554332	-2.052516	-0.015156	0.8251		31	999.753961	-999.753961
32	1049.426126	0.946143	-0.018029	0.8540		32	950.501816	-2.068292	-0.015776	0.8345		32		0.000000
33	1050.372269	0.928659	-0.017484	0.8813		33	948.433524	-2.083455	-0.015163	0.8783				
34	1051.300928	0.910911	-0.017748	0.9094		34	946.350069	-2.098209	-0.014754	0.8372				
35	1052.211839	0.893161	-0.017750	0.9094		35	944.251860	-2.112921	-0.014712	0.9176				
36	1053.105000	0.874665	-0.018496		Spl	36	942.138939	-2.127199	-0.014278	0.9241				
37	1053.979665	0.855652	-0.019013	0.9741		37	940.011740	-2.141526	-0.014327	0.9493				
38	1054.835317	##########	-1055.690969	0.9364	*	38	937.870214	-937.870214	-935.728688	0.9327				
						39								

			Calculated	Observed				Ground State Vco=0		Excited State Vco=1		
			R-P Diff	R-P Diff	R-P Diff	Δ1(R-P)	Δ2(R-P)	R(J) a-Type Frequencies		R(J) a-Type Frequencies		
Δ2	Int.	J	R(J)-P(J+2)	R(J)-P(J+2)	Obs-Calc			R(J)-Q(J+1)	Q(J)-P(J+1)	R(J)-Q(J)	Q(J+1)-P(J+1)	J
	0.0336	6	23.18565	23.186458	0.00081	0.00010		10.820792	10.818709	10.703187	10.701104	6
-0.018505	0.1255	7	26.27523	26.276138	0.00091	0.00032	0.00022	12.365776	12.365666	12.229666	12.229556	7
-0.016984	0.1673	8	29.36411	29.365334	0.00122	-0.00019	-0.00051	13.910580	13.910362	13.757486	13.757268	8
-0.017126	0.2329	9	32.45221	32.453243	0.00103	0.00016	0.00035	15.454667	15.454754	15.284447	15.284534	9
-0.016719	0.3144	10	35.53947	35.540661	0.00119	-0.00059	-0.00075	16.998388	16.998576	16.811449	16.811637	10
-0.017874	0.3316	11	38.62578	38.626379	0.00060	-0.00013	0.00046	18.541782	18.542273	18.336969	18.337460	11
-0.016071	0.2212	12	41.71108	41.711551	0.00047	0.00080	0.00093	20.083802	20.084597	19.862918	19.863713	12
-0.017446	0.4903	13	44.79527	44.796545	0.00127	0.00052	-0.00028	21.627360	21.627749	21.389030	21.389419	13
-0.016968	0.5388	14	47.87829	47.880087	0.00180	-0.00052	-0.00105	23.169622	23.169185	22.914324	22.913887	14
-0.017039	0.4479	15	50.96004	50.961313	0.00127	0.00009	0.00062	24.710293	24.710465	24.437956	24.438128	15
-0.017250	0.6062	16	54.04044	54.041806	0.00137	-0.00012	-0.00021	26.251121	26.251020	25.961534	25.961433	16
-0.016634	0.6731	17	57.11943	57.120677	0.00125	-0.00003	0.00009	27.790693	27.790685	27.484472	27.484464	17
-0.017842	0.5728	18	60.19690	60.198114	0.00121	-0.00005	-0.00002	29.330406	29.329984	29.006343	29.005921	18
-0.016134	0.7333	19	63.27278	63.273944	0.00116	-0.00006	-0.00001	30.868441	30.867708	30.528244	30.527511	19
-0.016931	0.7895	20	66.34700	66.348104	0.00110	0.00005	0.00011	32.405580	32.405503	32.048452	32.048375	20
-0.017693	0.8301	21	69.41946	69.420613	0.00115	-0.00063	-0.00068	33.942618	33.942524	33.567797	33.567703	21
-0.014935	0.8666	22	72.49009	72.490609	0.00052	0.00051	0.00114	35.476092	35.477995	35.086336	35.088239	22
-0.020953	0.5884	23	75.55881	75.559838	0.00103	-0.00051	-0.00102	37.013317	37.014517	36.602608	36.603808	23
-0.016087	0.8760	24	78.62552	78.626041	0.00052	-0.00005	0.00046	38.548350	38.546521	38.121554	38.119725	24
-0.013952	0.8804	25	81.69016	81.690634	0.00047	-0.00099	-0.00094	40.079102	40.077691	39.638354	39.636943	25
-0.020860	0.9436	26	84.75265	84.752135	-0.00051	0.00050	0.00149	41.612358	41.611532	41.150750	41.149924	26
-0.012641	0.6251	27	87.81289	87.812875	-0.00002	-0.00039	-0.00089	43.141628	43.139777	42.667379	42.665528	27
-0.018864	0.8969	28	90.87080	90.870394	-0.00041	-0.00079	-0.00040	44.670579	44.671247	44.177466	44.178134	28
-0.016829	0.9565	29	93.92632	93.925126	-0.00119	0.00006	0.00085	46.197893	46.199815	45.687951	45.689873	29
-0.017662	0.9588	30	96.97935	96.978217	-0.00113	-0.00025	-0.00031	47.726072	47.727233	47.198468	47.199629	30
-999.226357	0.9385	31	100.02981	100.028430	-0.00138	-0.00019	0.00005	##########	49.252145	48.707993	-950.501816	31
999.753961		32	103.07763	103.076057	-0.00157	-0.00073	-0.00054	##########	-948.433524	##########	-948.433524	32
		33	106.12271	106.120409	-0.00230	-0.00070	0.00003	##########	-946.350069	##########	-946.350069	33
		34	109.16499	109.161989	-0.00300	-0.00127	-0.00057					34
		35	112.20437	112.200099	-0.00427	-0.00171	-0.00044					35
		36	115.24077	115.234786	-0.00598	-118.26815	-118.26643					36
		37	118.27413		-118.27413							
		38	121.30434									

O-18 Methanol K=3 E2 n=0 (023)														
	R Branch	[Series G]					P Branch	[Series G]					Q Branch	
J	R(J)	Δ1	Δ2	Int.	C	J	P(J)	Δ1	Δ2	Int.	C	J	Q(J)	Δ1
	1008.046327						1008.046979						1008.046143	
3	1014.063795	1.462042		0.7035		3						3	1007.945043	-0.067400
4	1015.525837	1.445112	-0.016930	0.5495		4	1001.758869	-1.613570		0.6251	*	4	1007.877643	-0.084096
5	1016.970949	1.428034	-0.017078	0.4476		5	1000.145299	-1.630187	-0.016617	0.5447		5	1007.793547	-0.100760
6	1018.398983	1.410948	-0.017086	0.3843		6	998.515112	-1.646813	-0.016626	0.4588		6	1007.692787	-0.115406
7	1019.809931	1.393699	-0.017249	0.0954	*	7	996.868299	-1.663408	-0.016595	0.3980		7	1007.577381	-0.137444
8	1021.203630	1.376558	-0.017141	0.3133		8	995.204891	-1.679991	-0.016583	0.3457		8	1007.439937	-0.151527
9	1022.580188	1.359246	-0.017312	0.2943		9	993.524900	-1.696531	-0.016540	0.2112G*	*	9	1007.288410	-0.168356
10	1023.939434	1.341988	-0.017258	0.2786		10	991.828369	-1.713028	-0.016497	0.2956		10	1007.120054	-0.184881
11	1025.281422	1.324591	-0.017397	0.2773		11	990.115341	-1.729529	-0.016501	0.2863		11	1006.935173	-0.202730
12	1026.606013	1.307208	-0.017383	0.2407		12	988.385812	-1.745999	-0.016470	0.2854		12	1006.732443	-0.220074
13	1027.913221	1.289779	-0.017429	0.2827		13	986.639813	-1.762406	-0.016407	0.2796		13	1006.512369	-0.235163
14	1029.203000	1.272180	-0.017599	0.1796G*		14	984.877407	-1.778985	-0.016579	0.2889		14	1006.277206	-0.253645
15	1030.475180	1.254620	-0.017560	0.3062		15	983.098422	-1.795268	-0.016283	0.0907	*	15	1006.023561	-0.269397
16	1031.729800	1.236928	-0.017692	0.1076G*	*	16	981.303154	-1.811660	-0.016392	0.2983		16	1005.754164	-0.284456
17	1032.966728	1.219372	-0.017556	0.1035	*	17	979.491494	-1.828076	-0.016416	0.3183		17	1005.469708	-0.302766
18	1034.186100	1.201617	-0.017755	0.2876G*	*	18	977.663418	-1.844396	-0.016320	0.3584		18	1005.166942	##########
19	1035.387717	1.183786	-0.017831	0.4032		19	975.819022	-1.860742	-0.016346	0.4035		19		0.000000
20	1036.571503	1.165913	-0.017873	0.4401		20	973.958280	-1.877103	-0.016361	0.4365		20		0.000000
21	1037.737416	1.148132	-0.017781	0.4887		21	972.081177	-1.893440	-0.016337	0.4572		21		0.000000
22	1038.885548	1.129947	-0.018185	0.5173		22	970.187737	-1.909785	-0.016345	0.5094		22		0.000000
23	1040.015495	1.111996	-0.017951	0.5467		23	968.277952	-1.926099	-0.016314	0.5449		23		0.000000
24	1041.127491	1.093950	-0.018046	0.6174		24	966.351853	-1.942369	-0.016270	0.6024		24		0.000000
25	1042.221441	1.075936	-0.018014	0.6198		25	964.409484	-1.958727	-0.016358	0.6345		25		0.000000
26	1043.297377	1.057627	-0.018309	0.6524		26	962.450757	-1.975040	-0.016313	0.6767		26		0.000000
27	1044.355004	1.039496	-0.018131	0.7231		27	960.475717	-1.991359	-0.016319	0.7194		27		0.000000
28	1045.394500	1.021200	-0.018296	0.6003G*	*	28	958.484358	-2.007773	-0.016414	0.7479		28		0.000000
29	1046.415700	1.002976	-0.018224	0.8050		29	956.476585	-2.023982	-0.016209	0.7879		29		0.000000
30	1047.418676	0.984776	-0.018200	0.7775		30	954.452603	-2.040600	-0.016618	0.8228		30		0.000000
31	1048.403452	0.966106	-0.018670	0.8629		31	952.412003	-2.057004	-0.016404	0.8533		31		0.000000
32	1049.369558	0.947687	-0.018419	0.8866		32	950.354999	-2.073563	-0.016559	0.8786		32		
33	1050.317245	0.930000	-0.017687	0.8838		33	948.281436	-2.090213	-0.016650	0.9040				
34	1051.247245	0.911566	-0.018434	0.9050		34	946.191223	-2.106787	-0.016574	0.8990				
35	1052.158811	0.892818	-0.018748	0.9353		35	944.084436	-2.123929	-0.017142	0.9375				
36	1053.051629	0.875445	-0.017373	0.8666	*	36	941.960507	-2.140912	-0.016983	0.9445				
37	1053.927074	0.857227	-0.018218	0.9217	*	37	939.819595	-2.157987	-0.017075	0.9547				
38	1054.784301	0.836625	-0.020602	0.9639		38	937.661608	-2.175907	-0.017920	0.9537				
39	1055.620926	##########	-1056.457551	0.9247	*	39	935.485701	-935.485701	-933.309794	0.9477				

			Calculated	Observed				Ground State Vco=0		Excited State Vco=1		
			R-P Diff	R-P Diff	R-P Diff	Δ1(R-P)	Δ2(R-P)	R(J) a-Type Frequencies		R(J) a-Type Frequencies		
Δ2	Int.	J	R(J)-P(J+2)	R(J)-P(J+2)	Obs-Calc			R(J)-Q(J+1)	Q(J)-P(J+1)	R(J)-Q(J)	Q(J+1)-P(J+1)	J
	0.3599	3	13.91840	13.918496	0.00010	-0.00008		6.186152	6.186174	6.118752	6.118774	3
-0.016696	0.4459	4	17.01071	17.010725	0.00001	0.00001	0.00009	7.732290	7.732344	7.648194	7.648248	4
-0.016664	0.5444	5	20.10263	20.102650	0.00002	0.00000	0.00000	9.278162	9.278435	9.177402	9.177675	5
-0.014646	0.1227	6	23.19407	23.194092	0.00002	0.00004	0.00004	10.821602	10.824488	10.706196	10.709082	6
-0.022038	0.2985	7	26.28497	26.285031	0.00006	-0.00005	-0.00009	12.369994	12.372490	12.232550	12.235046	7
-0.014083	0.1881	8	29.37525	29.375261	0.00001	-0.00001	0.00004	13.915220	13.915037	13.763693	13.763510	8
-0.016829	0.1912	9	32.46485	32.464847	0.00000	-0.00006	-0.00004	15.460134	15.460041	15.291778	15.291685	9
-0.016525	0.7791	10	35.55368	35.553622	-0.00006	-0.00001	0.00004	17.004261	17.004713	16.819380	16.819832	10
-0.017849	0.6206	11	38.64168	38.641609	-0.00007	-0.00009	-0.00008	18.548979	18.549361	18.346249	18.346631	11
-0.017344	0.8354	12	41.72877	41.728606	-0.00016	0.00007	0.00017	20.093644	20.092630	19.873570	19.872556	12
-0.015089	0.5308	13	44.81489	44.814799	-0.00009	-0.00001	-0.00009	21.636015	21.634962	21.400852	21.399799	13
-0.018482	0.8780	14	47.89995	47.899846	-0.00010	-0.00010	-0.00009	23.179439	23.178784	22.925794	22.925139	14
-0.015752	0.8001	15	50.98389	50.983686	-0.00020	-0.00005	0.00005	24.721016	24.720407	24.451619	24.451010	15
-0.015059	0.5057	16	54.06664	54.066382	-0.00026	-0.00015	-0.00009	26.260092	26.262670	25.975636	25.978214	16
-0.018310	0.8661	17	57.14811	57.147706	-0.00040	-0.00003	0.00012	27.799786	27.806290	27.497020	27.503524	17
-1004.864176	0.8626	18	60.22825	60.227820	-0.00043	0.00000	0.00003	##########	29.347920	29.019158	-975.819022	18
1005.166942		19	63.30697	63.306540	-0.00043	0.00000	0.00000	##########	-973.958280	##########	-973.958280	19
0.000000		20	66.38420	66.383766	-0.00043	0.00002	0.00002	##########	-972.081177	##########	-972.081177	20
0.000000		21	69.45988	69.459464	-0.00042	0.00019	0.00017	##########	-970.187737	##########	-970.187737	21
0.000000		22	72.53392	72.533695	-0.00023	-0.00003	-0.00022	##########	-968.277952	##########	-968.277952	22
0.000000		23	75.60627	75.606011	-0.00026	0.00016	0.00020	##########	-966.351853	##########	-966.351853	23
0.000000		24	78.67683	78.676734	-0.00010	0.00027	0.00011	##########	-964.409484	##########	-964.409484	24
0.000000		25	81.74555	81.745724	0.00017	0.00051	0.00024	##########	-962.450757	##########	-962.450757	25
0.000000		26	84.81234	84.813019	0.00068	0.00059	0.00008	##########	-960.475717	##########	-960.475717	26
0.000000		27	87.87715	87.878419	0.00127	0.00075	0.00016	##########	-958.484358	##########	-958.484358	27
0.000000		28	90.93988	90.941897	0.00202	0.00120	0.00045	##########	-956.476585	##########	-956.476585	28
0.000000		29	94.00048	94.003697	0.00322	0.00159	0.00039	##########	-954.452603	##########	-954.452603	29
0.000000		30	97.05887	97.063677	0.00481	0.00224	0.00065	##########	-952.412003	##########	-952.412003	30
0.000000		31	100.11497	100.122016	0.00705	0.00257	0.00033	##########	-950.354999	##########	-950.354999	31
		32	103.16872	103.178335	0.00962	0.00315	0.00058	##########	-948.281436	##########	-948.281436	32
		33	106.22004	106.232809	0.01277	0.00511	0.00196					33
		34	109.26886	109.286738	0.01788	0.00624	0.00113					34
		35	112.31510	112.339216	0.02412	0.00721	0.00097					35
		36	115.35870	115.390021	0.03132	0.01047	0.00327					36
		37	118.39958	118.441373	0.04179	933.30484	933.29437					
		38	121.43767	##########	933.34663	122.27430	-811.03054					
		39		##########	1055.62093	-1055.62093	-1177.89522					
					0.00000							

O-18 Methanol K=4 E1 n=0 (024)

	R Branch	[Series I]					P Branch	[Series I]					Q Branch	
J	R(J)	Δ1	Δ2	Int.	C	J	P(J)	Δ1	Δ2	Int.	C	J	Q(J)	Δ1
	1008.096368						1008.099169						1008.089203	
4	1015.573578	1.444535		0.7245		4						4	1007.924363	-0.082420
5	1017.018113	1.427566	-0.016969	0.5955		5	1000.194709	-1.630461		0.7111		5	1007.841943	-0.101743
6	1018.445679	1.410012	-0.017554	0.4666		6	998.564248	-1.646984	-0.016523	0.5795		6	1007.740200	-0.117863
7	1019.855691	1.393535	-0.016477	0.4017		7	996.917264	-1.663689	-0.016705	0.5041		7	1007.622337	-0.134776
8	1021.249226	1.376004	-0.017531	0.2994		8	995.253575	-1.680275	-0.016586	0.4012		8	1007.487561	-0.152346
9	1022.625230	1.358654	-0.017350	0.3554		9	993.573300	-1.696995	-0.016720	0.3843		9	1007.335215	-0.168208
10	1023.983884	1.341201	-0.017453	0.3373		10	991.876305	-1.714050	-0.017055	0.3520		10	1007.167007	-0.186612
11	1025.325085	1.324044	-0.017157	0.1976		11	990.162255	-1.729513	-0.015463	0.2461		11	1006.980395	-0.202886
12	1026.649129	1.306507	-0.017537	0.3219		12	988.432742	-1.746623	-0.017110	0.3427		12	1006.777509	-0.220035
13	1027.955636	1.288914	-0.017593	0.3361		13	986.686119	-1.763147	-0.016524	0.3136		13	1006.557474	-0.235935
14	1029.244550	1.271461	-0.017453	0.3251		14	984.922972	-1.780327	-0.017180	0.3434		14	1006.321539	-0.251828
15	1030.516011	1.253892	-0.017569	0.3499		15	983.142645	-1.795463	-0.015136	0.1342		15	1006.069711	-0.277188
16	1031.769903	1.236393	-0.017499	0.3785		16	981.347182	-1.812658	-0.017195	0.3773		16	1005.792523	##########
17	1033.006296	1.218254	-0.018139	0.3212		17	979.534524	-1.829026	-0.016368	0.3621		17		0.000000
18	1034.224550	1.200724	-0.017530	0.4305		18	977.705498	-1.845481	-0.016455	0.4227		18		0.000000
19	1035.425274	1.182257	-0.018467	0.4588		19	975.860017	-1.861974	-0.016493	0.4532		19		0.000000
20	1036.607531	1.165616	-0.016641	0.2257		20	973.998043	-1.878553	-0.016579	0.4814		20		0.000000
21	1037.773147	1.147010	-0.018606	0.5326		21	972.119490	-1.894462	-0.015909	0.2435		21		0.000000
22	1038.920157	1.129073	-0.017937	0.5802		22	970.225028	-1.911141	-0.016679	0.5462		22		0.000000
23	1040.049230	1.110966	-0.018107	0.6033		23	968.313887	-1.927534	-0.016393	0.5947		23		0.000000
24	1041.160196	1.092687	-0.018279	0.6393		24	966.386353	-1.943797	-0.016263	0.6325		24		0.000000
25	1042.252883	1.075765	-0.016922	0.6892		25	964.442556	-1.960349	-0.016552	0.6688		25		0.000000
26	1043.328648	1.055069	-0.020696	0.4871		26	962.482207	-1.975305	-0.014956	0.7116		26		0.000000
27	1044.383717	1.037943	-0.017126	0.7028		27	960.506902	-1.994178	-0.018873	0.6427		27		0.000000
28	1045.421660	1.019525	-0.018418	0.7635		28	958.512724	-2.009391	-0.015213	0.7732		28		0.000000
29	1046.441185	1.000948	-0.018577	0.8070		29	956.503333	-2.025718	-0.016327	0.8131		29		0.000000
30	1047.442133	0.982467	-0.018481	0.8505		30	954.477615	-2.041992	-0.016274	0.8525		30		0.000000
31	1048.424600	0.963486	-0.018981	0.8588		31	952.435623	-2.058411	-0.016419	0.8716		31		0.000000
32	1049.388086	0.944178	-0.019308	0.8906		32	950.377212	-2.074858	-0.016447	0.8952		32		
33	1050.332264	0.925774	-0.018404	0.8998		33	948.302354	-2.091401	-0.016543	0.9170				
34	1051.258038	0.906980	-0.018794	0.9221		34	946.210953	-2.107825	-0.016424	0.9272				
35	1052.165018	0.886611	-0.020369	0.8738		35	944.103128	-2.124221	-0.016396	0.9344				
36	1053.051629	0.872371	-0.014240	0.8664	•	36	941.978907	-2.141770	-0.017549	0.9523				
37	1053.924000	0.851411	-0.020960			37	939.837137	-2.159137	-0.017367	0.9526				
38	1054.775411	##########	-1055.626822	0.9646		38	937.678000	-937.678000	-935.518863					

			Calculated	Observed				Ground State Vco=0		Excited State Vco=1		
			R-P Diff	R-P Diff	R-P Diff	Δ1(R-P)	Δ2(R-P)	R(J) a-Type Frequencies		R(J) a-Type Frequencies		
Δ2	Int.	J	R(J)-P(J+2)	R(J)-P(J+2)	Obs-Calc			R(J)-Q(J+1)	Q(J)-P(J+1)	R(J)-Q(J)	Q(J+1)-P(J+1)	J
	0.0318	4	17.00909	17.009330	0.00024	-0.00015		7.731635	7.729654	7.649215	7.647234	4
-0.019323	0.3818	5	20.10076	20.100849	0.00009	0.00004	0.00019	9.277913	9.277695	9.176170	9.175952	5
-0.016120	0.3913	6	23.19198	23.192104	0.00012	-0.00041	-0.00045	10.823342	10.822936	10.705479	10.705073	6
-0.016913	0.5356	7	26.28268	26.282391	-0.00029	0.00041	0.00082	12.368130	12.368762	12.233354	12.233986	7
-0.017570	0.3467	8	29.37280	29.372921	0.00012	0.00058	0.00017	13.914011	13.914261	13.761665	13.761915	8
-0.015862	0.6389	9	32.46227	32.462975	0.00071	-0.00057	-0.00116	15.458223	15.458910	15.290015	15.290702	9
-0.018404	0.5241	10	35.55101	35.551142	0.00013	-0.00012	0.00046	17.003489	17.004752	16.816877	16.818140	10
-0.016274	0.7225	11	38.63895	38.638966	0.00002	0.00010	0.00022	18.547576	18.547653	18.344690	18.344767	11
-0.017149	0.5378	12	41.72604	41.726157	0.00012	0.00067	0.00057	20.091655	20.091390	19.871620	19.871355	12
-0.015900	0.7861	13	44.81220	44.812991	0.00079	-0.00078	-0.00146	21.634097	21.634502	21.398162	21.398567	13
-0.015893	0.4671	14	47.89736	47.897368	0.00001	0.00003	0.00081	23.174839	23.178894	22.923011	22.927066	14
-0.025360	0.6521	15	50.98145	50.981487	0.00004	-0.00003	-0.00006	24.723488	24.722529	24.446300	24.445341	15
-1005.515335	0.4921	16	54.06440	54.064405	0.00001	0.00012	0.00016	##########	26.257999	25.977380	-979.534524	16
1005.792523		17	57.14615	57.146279	0.00013	-0.00025	-0.00038	##########	-977.705498	##########	-977.705498	17
0.000000		18	60.22663	60.226507	-0.00012	0.00015	0.00040	##########	-975.860017	##########	-975.860017	18
0.000000		19	63.30576	63.305784	0.00002	-0.00100	-0.00115	##########	-973.998043	##########	-973.998043	19
0.000000		20	66.38348	66.382503	-0.00098	0.00052	0.00152	##########	-972.119490	##########	-972.119490	20
0.000000		21	69.45972	69.459260	-0.00046	-0.00015	-0.00066	##########	-970.225028	##########	-970.225028	21
0.000000		22	72.53441	72.533804	-0.00061	-0.00020	-0.00005	##########	-968.313887	##########	-968.313887	22
0.000000		23	75.60748	75.606674	-0.00081	-0.00007	0.00013	##########	-966.386353	##########	-966.386353	23
0.000000		24	78.67886	78.677989	-0.00087	-0.00164	-0.00157	##########	-964.442556	##########	-964.442556	24
0.000000		25	81.74849	81.745981	-0.00251	0.00214	0.00378	##########	-962.482207	##########	-962.482207	25
0.000000		26	84.81629	84.815924	-0.00037	-0.00145	-0.00359	##########	-960.506902	##########	-960.506902	26
0.000000		27	87.88220	87.880384	-0.00182	-0.00028	0.00117	##########	-958.512724	##########	-958.512724	27
0.000000		28	90.94614	90.944045	-0.00210	-0.00040	-0.00012	##########	-956.503333	##########	-956.503333	28
0.000000		29	94.00806	94.005562	-0.00250	-0.00045	-0.00005	##########	-954.477615	##########	-954.477615	29
0.000000		30	97.06787	97.064921	-0.00295	-0.00032	0.00014					30
0.000000		31	100.12551	100.122246	-0.00326	-0.00052	-0.00021					31
		32	103.18092	103.177133	-0.00379	-0.00110	-0.00057					32
		33	106.23402	106.229136	-0.00488	-0.00073	0.00037					33
		34	109.28474	109.279131	-0.00561	0.00048	0.00121					34
		35	112.33301	112.327881	-0.00513	-0.00001	-0.00049					35
		36	115.37877	115.373629	-0.00514	-118.41681	-118.41680					36
		37	118.42195		-118.42195							
		38	121.46248									

O-18 Methanol K=6 E2 n=0 (026)

	R Branch	[Series Q]					P Branch	[Series Q]					Q Branch	
J	R(J)	Δ1	Δ2	Int.	C	J	P(J)	Δ1	Δ2	Int.	C	J	Q(J)	Δ1
	1008.346975						1008.208710						1008.256296	
6	1018.599756	1.407003		0.2171	*	6						6	1007.898426	-0.119290
7	1020.006759	1.392583	-0.014420	0.1930	*	7	997.078227	-1.664461		0.8030		7	1007.779136	-0.136515
8	1021.399342	1.374351	-0.018232	0.5942		8	995.413766	-1.683059	-0.018598	0.6982		8	1007.642621	-0.155060
9	1022.773693	1.356446	-0.017905	0.4784	*	9	993.730707	-1.696044	-0.012985	0.5771	*	9	1007.487561	-0.168933
10	1024.130139	1.338909	-0.017537	0.1195	*	10	992.034663	-1.716389	-0.020345	0.5565		10	1007.318628	-0.187477
11	1025.469048	1.321728	-0.017181	0.4913		11	990.318274	-1.729739	-0.013350	0.1841	*	11	1007.131151	-0.204641
12	1026.790776	1.304238	-0.017490	0.4899		12	988.588535	-1.748042	-0.018303	0.5093		12	1006.926510	-0.221680
13	1028.095014	1.286769	-0.017469	0.4374		13	986.840493	-1.764247	-0.016205	0.5072		13	1006.704830	-0.237402
14	1029.381783	1.269184	-0.017585	0.4938	*	14	985.076246	-1.781590	-0.017343	0.4258	*	14	1006.467428	-0.257435
15	1030.650967	1.251880	-0.017304	0.4887		15	983.294656	-1.797771	-0.016181	0.5087		15	1006.209993	-0.272774
16	1031.902847	1.235052	-0.016828	0.1624	*	16	981.496885	-1.814202	-0.016431	0.5204		16	1005.937219	-0.289524
17	1033.137899	1.215119	-0.019933	0.2627	*	17	979.682683	-1.830836	-0.016634	0.5030		17	1005.647695	-0.306822
18	1034.353018	1.198696	-0.016423	0.5346		18	977.851847	-1.847173	-0.016337	0.5455		18	1005.340873	-0.325178
19	1035.551714	1.181025	-0.017671	0.5843		19	976.004674	-1.863620	-0.016447	0.5711	*	19	1005.015695	-0.339877
20	1036.732739	1.163277	-0.017748	0.5161		20	974.141054	-1.879878	-0.016258	0.5822		20	1004.675818	-0.357799
21	1037.896016	1.145512	-0.017765	0.6426		21	972.261176	-1.896263	-0.016385	0.6385		21	1004.318019	-0.376334
22	1039.041528	1.127826	-0.017686	0.6799		22	970.364913	-1.912585	-0.016322	0.6458		22	1003.941685	-0.387782
23	1040.169354	1.109968	-0.017858	0.7054		23	968.452328	-1.928695	-0.016110	0.6945		23	1003.553903	-0.411918
24	1041.279322	1.092188	-0.017780	0.7362	LC	24	966.523633	-1.945033	-0.016338	0.7233		24	1003.141985	-0.425565
25	1042.371510	1.074439	-0.017749	0.7655		25	964.578600	-1.959526	-0.014493	0.7460		25	1002.716420	-0.446323
26	1043.445949	1.056332	-0.018107	0.8009		26	962.619074	-1.979100	-0.019574	0.6670	*	26	1002.270097	-0.456867
27	1044.502281	1.039503	-0.016829	0.8057		27	960.639974	-1.993771	-0.014671	0.6190	*	27	1001.813230	-0.475465
28	1045.541784	1.022379	-0.017124	0.8413		28	958.646203	-2.007918	-0.014147	0.6780	*	28	1001.337765	-0.490329
29	1046.564163	1.000122	-0.022257	0.6944	*	29	956.638285	-2.024844	-0.016926	0.8651		29	1000.847436	##########
30	1047.564285	0.990047	-0.010075	0.7798	*	30	954.613441	-2.040132	-0.015268	0.8814		30		0.000000
31	1048.554332	0.970925	-0.019122	0.9149		31	952.573309	-2.055522	-0.015390	0.9040		31		0.000000
32	1049.525257	0.953614	-0.017311	0.7627	*	32	950.517787	-2.070460	-0.014938	0.9117		32		
33	1050.478871	##########	-1051.432485	0.9586		33	948.447327	-2.087019	-0.016559	0.9348				
34		0.000000	1050.478871			34	946.360308	-2.097515	-0.010496	0.9049				
35		0.000000	0.000000			35	944.262793	-2.115179	-0.017664	0.9634				
36		0.000000	0.000000			36	942.147614	-942.147614	-940.032435	0.9649				

			Calculated	Observed				Ground State Vco=0		Excited State Vco=1		
			R-P Diff	R-P Diff	R-P Diff	Δ1(R-P)	Δ2(R-P)	R(J) a-Type Frequencies		R(J) a-Type Frequencies		
Δ2	Int.	J	R(J)-P(J+2)	R(J)-P(J+2)	Obs-Calc			R(J)-Q(J+1)	Q(J)-P(J+1)	R(J)-Q(J)	Q(J+1)-P(J+1)	J
	0.2881	6	23.18510	23.185990	0.00089	0.00021		10.820620	10.820199	10.701330	10.700909	6
-0.017225	0.3342	7	26.27495	26.276052	0.00110	-0.00065	-0.00086	12.364138	12.365370	12.227623	12.228855	7
-0.018545	0.4071	8	29.36423	29.364679	0.00045	0.00210	0.00275	13.911781	13.911914	13.756721	13.756854	8
-0.013873	0.3467	9	32.45287	32.455419	0.00255	-0.00176	-0.00386	15.455065	15.452898	15.286132	15.283965	9
-0.018544	0.5513	10	35.54082	35.541604	0.00078	-0.00024	0.00153	16.998988	17.000354	16.811511	16.812877	10
-0.017164	0.5469	11	38.62801	38.628555	0.00054	-0.00038	-0.00015	18.542538	18.542616	18.337897	18.337975	11
-0.017039	0.6473	12	41.71437	41.714530	0.00016	0.00037	0.00075	20.085946	20.086017	19.864266	19.864337	12
-0.015722	0.6921	13	44.79983	44.800358	0.00053	0.00004	-0.00033	21.627586	21.628584	21.390184	21.391182	13
-0.020033	0.4906	14	47.88433	47.884898	0.00057	-0.00008	-0.00012	23.171790	23.172772	22.914355	22.915337	14
-0.015339	0.7391	15	50.96780	50.968284	0.00048	0.00034	0.00042	24.713748	24.713108	24.440974	24.440334	15
-0.016750	0.5515	16	54.05018	54.051000	0.00082	0.00101	0.00068	26.255152	26.254536	25.965628	25.965012	16
-0.017298	0.7970	17	57.13139	57.133225	0.00184	-0.00125	-0.00227	27.797026	27.795848	27.490204	27.489026	17
-0.018356	0.8596	18	60.21136	60.211964	0.00058	-0.00012	0.00114	29.337323	29.336199	29.012145	29.011021	18
-0.014699	0.8390	19	63.29007	63.290538	0.00047	-0.00005	0.00006	30.875896	30.874641	30.536019	30.534764	19
-0.017922	0.8996	20	66.36741	66.367826	0.00042	-0.00004	0.00001	32.414720	32.414642	32.056921	32.056843	20
-0.018535	0.8707	21	69.44331	69.443688	0.00038	-0.00020	-0.00016	33.954331	33.953106	33.577997	33.576772	21
-0.011448	0.8742	22	72.51772	72.517895	0.00017	0.00001	0.00021	35.487625	35.489357	35.099843	35.101575	22
-0.024136	0.9361	23	75.59057	75.590754	0.00018	-0.00174	-0.00175	37.027369	37.030270	36.615451	36.618352	23
-0.013647	0.9462	24	78.66180	78.660248	-0.00155	0.00176	0.00349	38.562902	38.563385	38.137337	38.137820	24
-0.020758	0.9692	25	81.73133	81.731536	0.00021	0.00043	-0.00133	40.101413	40.097346	39.655090	39.651023	25
-0.010544	0.9321	26	84.79911	84.799746	0.00064	-0.00170	-0.00213	41.632719	41.630123	41.175852	41.173256	26
-0.018598	0.9750	27	87.86506	87.863996	-0.00106	0.00029	0.00199	43.164516	43.167027	42.689051	42.691562	27
-0.014864	0.9559	28	90.92912	90.928343	-0.00078	0.00041	0.00012	44.694348	44.699480	44.204019	44.209151	28
-1000.357107	0.9648	29	93.99122	93.990854	-0.00037	-0.00443	-0.00484	##########	46.233995	45.716727	-954.613441	29
1000.847436		30	97.05129	97.046498	-0.00479	0.00252	0.00694					30
0.000000		31	100.10928	100.107005	-0.00228	0.00212	-0.00039					31
		32	103.16510	103.164949	-0.00015	-0.00248	-0.00460					32
		33	106.21871	106.216078	-0.00263	-1051.41500	-1051.41252					33
		34	109.27002	-942.147614	-1051.41763	939.09865	1990.51366					34
		35	112.31898	0.000000	-112.31898	-3.04654	-942.14519					35
		36	115.36552	0.000000	-115.36552	-3.04405	0.00249					36
		37	118.40957		-118.40957							
		38	121.45106									

O-18 Methanol C-O K=0 E n=0 (030) E																
											Calculated					
	R Branch					P Branch					R-P Diff	R-P Diff	R-P Diff	Δ1(R-P)	Δ2(R-P)	R-P Diff
J	R(J)	Δ1	Δ2	Int.	J	P(J)	Δ1	Δ2	Int.	J	R(J)-P(J+2)	R(J)-P(J+2)	Obs-Calc			MW Obsvns
	1008.062288					1008.061777										
0	1009.592387	1.512809		0.7856						0	4.63982	4.639842	0.00002	-0.00005		4.639810
1	1011.105196	1.495519	-0.017290	0.6224	1	1006.515450	-1.562905		0.6713	1	7.73216	7.732134	-0.00003	-0.00007	-0.00002	7.732147
2	1012.600715	1.478045	-0.017474	0.4976	2	1004.952545	-1.579483	-0.016578	0.6157	2	10.82318	10.823084	-0.00010	0.00020	0.00027	10.823179
3	1014.078760	1.460045	-0.018000	0.3856	3	1003.373062	-1.595431	-0.015948	0.4834	3	13.91237	13.912476	0.00011	-0.00008	-0.00029	
4	1015.538805	1.442071	-0.017974	0.3403	4	1001.777631	-1.611347	-0.015916	0.3713	4	16.99920	16.999222	0.00002	0.00010	0.00019	
5	1016.980876	1.423823	-0.018248	0.2925	5	1000.166264	-1.626701	-0.015354	0.3460	5	20.08314	20.083264	0.00012	0.00024	0.00013	
6	1018.404699	1.405232	-0.018591	0.2537	6	998.539583	-1.641971	-0.015270	0.2969	6	23.16367	23.164030	0.00036	0.00036	0.00013	
7	1019.809931	1.386657	-0.018575	0.0954	7	996.897612	-1.656943	-0.014972	0.2692	7	26.24026	26.240983	0.00072	0.00079	0.00043	
8	1021.196588	1.368456	-0.018201	0.1990	8	995.240669	-1.671721	-0.014778	0.2403	8	29.31240	29.313912	0.00151	0.00202	0.00123	
9	1022.565044	1.348414	-0.020042	0.0496	9	993.568948	-1.686272	-0.014551	0.2174	9	32.37954	32.383075	0.00353	0.00178	-0.00024	
10	1023.913458	1.329215	-0.019199	0.0686	10	991.882676	-1.700707	-0.014435	0.2166	10	35.44118	35.446498	0.00532	0.00303	0.00125	
11	1025.242673	1.310390	-0.018825	0.1930	11	990.181969	-1.715009	-0.014302	0.2061	11	38.49678	38.505132	0.00835	0.00518	0.00215	
12	1026.553063	1.291596	-0.018794	0.1900	12	988.466960	-1.729419	-0.014410	0.2085	12	41.54583	41.559363	0.01353	0.00795	0.00276	
13	1027.844659	1.272460	-0.019136	0.1988	13	986.737541	-1.743841	-0.014422	0.2117	13	44.58778	44.609259	0.02148	0.01091	0.00296	
14	1029.117119	1.253502	-0.018958	0.2134	14	984.993700	-1.758300	-0.014459	0.1727G*	14	47.62213	47.654519	0.03239	0.01458	0.00367	
15	1030.370621	1.234833	-0.018669	0.2298	15	983.235400	-1.772800	-0.014500	0.0759G*	15	50.64835	50.695321	0.04697	0.01978	0.00520	
16	1031.605454	1.216227	-0.018606	0.1779	16	981.462600	-1.787300	-0.014500	0.0938G*	16	53.66590	53.732653	0.06675	0.02575	0.00597	
17	1032.821681	1.197713	-0.018514	0.2516	17	979.675300	-1.802499	-0.015199	0.1754G*	17	56.67428	56.766787	0.09251	0.03244	0.00668	
18	1034.019394	1.179653	-0.018060	0.2794	18	977.872801	-1.817907	-0.015408	0.3052	18	59.67294	59.797885	0.12494	0.04033	0.00789	
19	1035.199047	1.161553	-0.018100	0.3442	19	976.054894	-1.833385	-0.015478	0.3346	19	62.66137	62.826647	0.16528	0.04888	0.00855	
20	1036.360600	1.143555	-0.017998	0.3292G*	20	974.221509	-1.849109	-0.015724	0.3738	20	65.63904	65.853200	0.21416	0.05816	0.00927	
21	1037.504155	1.125645	-0.017910	0.3868	21	972.372400	-1.865000	-0.015891	0.2134G*	21	68.60543	68.877747	0.27232	0.06815	0.00999	
22	1038.629800	1.107829	-0.017816	0.3470G*	22	970.507400	-1.880992	-0.015992	0.3030G*	22	71.56001	71.900474	0.34046	0.07889	0.01074	
23	1039.737629	1.090098	-0.017731	0.5068	23	968.626408	-1.897082	-0.016090	0.4925	23	74.50226	74.921612	0.41935	0.09029	0.01140	
24	1040.827727	1.072412	-0.017686	0.5389	24	966.729326	-1.913309	-0.016227	0.5427	24	77.43165	77.941291	0.50964	0.10217	0.01188	
25	1041.900139	1.054585	-0.017827	0.5924	25	964.816017	-1.929581	-0.016272	0.5823	25	80.34766	80.959473	0.61181	0.11434	0.01217	
26	1042.954724	1.036914	-0.017671	0.6486	26	962.886436	-1.945770	-0.016189	0.6376	26	83.24977	83.975924	0.72615	0.12735	0.01301	
27	1043.991638	1.019087	-0.017827	0.6709	27	960.940666	-1.961866	-0.016096	0.6838	27	86.13744	86.990942	0.85350	0.14074	0.01339	
28	1045.010725	1.001276	-0.017811	0.7052	28	958.978800	-1.978104	-0.016238	0.5656G*	28	89.01015	90.004390	0.99424	0.15430	0.01356	
29	1046.012001	0.983499	-0.017777	0.7699	29	957.000696	-1.994361	-0.016257	0.7508	29	91.86739	93.015931	1.14854	0.16869	0.01439	
30	1046.995500	0.965605	-0.017894	0.7459G*	30	955.006335	-2.010265	-0.015904	0.7939	30	94.70861	96.025845	1.31724	0.18314	0.01445	
31	1047.961105	0.947687	-0.017918	0.8248	31	952.996070	-2.026415	-0.016150	0.8253	31	97.53331	99.033688	1.50038	0.19814	0.01500	
32	1048.908792	0.929720	-0.017967	0.8514	32	950.969655	-2.042238	-0.015823	0.8585	32	100.34095	102.039467	1.69852	0.21359	0.01545	
33	1049.838512	0.911768	-0.017952	0.8770	33	948.927417	-2.058092	-0.015854	0.8656	33	103.13101	105.043112	1.91210	0.22931	0.01572	
34	1050.750280	0.893505	-0.018263	0.9008	34	946.869325	-2.073925	-0.015833	0.9044	34	105.90297	108.044379	2.14141	0.24528	0.01597	
35	1051.643785	0.876115	-0.017390	0.9205	35	944.795400	-2.089499	-0.015574	0.9168	35	108.65630	111.042985	2.38668	0.26282	0.01754	
36	1052.519900	0.857321	-0.018794	0.9346	36	942.705901	-2.105101	-0.015602	0.9304	36	111.39047	114.039974	2.64950			
37	1053.377221	0.840227	-0.017094	0.9544	37	940.600800	-2.120874	-0.015773	0.9395G*	37						
38	1054.217448	##########	-1055.057675	0.9542	38	938.479926	-938.479926	-936.359052	0.9509	38						
							0.000000	938.479926								

O-18 Methanol K=5 E2 n=0 (035)

	R Branch	[Series D]					P Branch	[Series D]					Q Branch	
J	R(J)	Δ1	Δ2	Int.	C	J	P(J)	Δ1	Δ2	Int.	C	J	Q(J)	Δ1
	1007.947680						1008.045989						1008.017478	
5	1016.935647	1.427823		0.7525		5						5	1007.762105	-0.102149
6	1018.363470	1.407774	-0.020049	0.2230	*	6	998.486477	-1.648139		0.7584		6	1007.659956	-0.119055
7	1019.771244	1.391835	-0.015939	0.5388		7	996.838338	-1.663821	-0.015682	0.1894	*	7	1007.540901	-0.136563
8	1021.163079	1.374718	-0.017117	0.4630		8	995.174517	-1.681219	-0.017398	0.5412		8	1007.404338	-0.153298
9	1022.537797	1.356909	-0.017809	0.3912	*	9	993.493298	-1.697869	-0.016650	0.4770		9	1007.251040	-0.172917
10	1023.894706	1.339857	-0.017052	0.3841	*	10	991.795429	-1.714657	-0.016788	0.4264		10	1007.078123	-0.184927
11	1025.234563	1.322407	-0.017450	0.3881		11	990.080772	-1.731541	-0.016884	0.3898		11	1006.893196	-0.203214
12	1026.556970	1.304775	-0.017632	0.3857		12	988.349231	-1.748136	-0.016595	0.3979		12	1006.689982	-0.222554
13	1027.861745	1.287316	-0.017459	0.3840		13	986.601095	-1.764769	-0.016633	0.3805		13	1006.467428	-0.238984
14	1029.149061	1.269753	-0.017563	0.3915		14	984.836326	-1.780444	-0.015675	0.3332		14	1006.228444	-0.253637
15	1030.418814	1.252379	-0.017374	0.4123		15	983.055882	-1.799284	-0.018840	0.1938	*	15	1005.974807	-0.273461
16	1031.671193	1.234256	-0.018123	0.2922		16	981.256598	-1.816869	-0.017585	0.1347	*	16	1005.701346	-0.291240
17	1032.905449	1.216726	-0.017530	0.4370		17	979.439729	-1.829323	-0.012454	0.0814	*	17	1005.410106	-0.305597
18	1034.122175	1.199070	-0.017656	0.4617		18	977.610406	-1.848023	-0.018700	0.4517		18	1005.104509	-0.324702
19	1035.321245	1.181244	-0.017826	0.4638		19	975.762383	-1.864610	-0.016587	0.5023		19	1004.779807	-0.340767
20	1036.502489	1.163292	-0.017952	0.4956		20	973.897773	-1.881189	-0.016579	0.5265		20	1004.439040	-0.358258
21	1037.665781	1.145341	-0.017951	0.5670		21	972.016584	-1.897713	-0.016524	0.5644		21	1004.080782	-0.375469
22	1038.811122	1.128060	-0.017281	0.5917		22	970.118871	-1.914331	-0.016618	0.5956		22	1003.705313	-0.394313
23	1039.939182	1.109391	-0.018669	0.3580	*	23	968.204540	-1.930755	-0.016424	0.6374		23	1003.311000	-0.408849
24	1041.048573	1.091782	-0.017609	0.6738		24	966.273785	-1.947333	-0.016578	0.6699		24	1002.902151	-0.429355
25	1042.140355	1.072958	-0.018824	0.7075		25	964.326452	-1.963811	-0.016478	0.6937		25	1002.472796	-0.441652
26	1043.213313	1.055536	-0.017422	0.7403		26	962.362641	-1.979934	-0.016123	0.7349		26	1002.031144	-0.464127
27	1044.268849	1.037226	-0.018310	0.7583		27	960.382707	-1.997160	-0.017226	0.7806		27	1001.567017	##########
28	1045.306075	1.019244	-0.017982	0.7042		28	958.385547	-2.013205	-0.016045	0.7715		28		0.000000
29	1046.325319	1.000979	-0.018265	0.8151		29	956.372342	-2.029581	-0.016376	0.8305		29		0.000000
30	1047.326298	0.982764	-0.018215	0.8570		30	954.342761	-2.045899	-0.016318	0.8657		30		0.000000
31	1048.309062	0.965046	-0.017718	0.8763		31	952.296862	-2.061792	-0.015893	0.8863		31		0.000000
32	1049.274108	0.947437	-0.017609	0.9191		32	950.235070	-2.078741	-0.016949	0.7860	*	32		
33	1050.221545	0.930219	-0.017218	0.9250		33	948.156329	-2.094354	-0.015613	0.9190				
34	1051.151764	0.912408	-0.017811	0.8653	*	34	946.061975	-2.109821	-0.015467	0.9310				
35	1052.064172	##########	-1052.976580	0.8951	*	35	943.952154	-2.123491	-0.013670	0.9478				
36		0.000000	1052.064172			36	941.828663	-941.828663	-939.705172	0.9484				

			Calculated	Observed				Ground State Vco=0		Excited State Vco=1		
			R-P Diff	R-P Diff	R-P Diff	Δ1(R-P)	Δ2(R-P)	R(J) a-Type Frequencies		R(J) a-Type Frequencies		
Δ2	Int.	J	R(J)-P(J+2)	R(J)-P(J+2)	Obs-Calc			R(J)-Q(J+1)	Q(J)-P(J+1)	R(J)-Q(J)	Q(J+1)-P(J+1)	J
	0.2267	5	20.09664	20.097309	0.00067	0.00088		9.275691	9.275628	9.173542	9.173479	5
-0.016906	0.3372	6	23.18740	23.188953	0.00155	-0.00132	-0.00220	10.822569	10.821618	10.703514	10.702563	6
-0.017508	0.3896	7	26.27771	26.277946	0.00024	-0.00011	0.00121	12.366906	12.366384	12.230343	12.229821	7
-0.016735	0.1550	8	29.36752	29.367650	0.00013	0.00012	0.00023	13.912039	13.911040	13.758741	13.757742	8
-0.019619	0.2040	9	32.45677	32.457025	0.00025	-0.00017	-0.00029	15.459674	15.455611	15.286757	15.282694	9
-0.012010	0.4048	10	35.54539	35.545475	0.00009	0.00004	0.00021	17.001510	16.997351	16.816583	16.812424	10
-0.018287	0.4112	11	38.63334	38.633468	0.00013	-0.00003	-0.00008	18.544581	18.543965	18.341367	18.340751	11
-0.019340	0.5648	12	41.72055	41.720644	0.00009	-0.00119	-0.00116	20.089542	20.088887	19.866988	19.866333	12
-0.016430	0.4906	13	44.80696	44.805863	-0.00110	0.00105	0.00224	21.633301	21.631102	21.394317	21.392118	13
-0.014653	0.4584	14	47.89251	47.892463	-0.00005	0.00199	0.00094	23.174254	23.172562	22.920617	22.918925	14
-0.019824	0.4623	15	50.97714	50.979085	0.00195	-0.00196	-0.00395	24.717468	24.718209	24.444007	24.444748	15
-0.017779	0.7723	16	54.06080	54.060787	-0.00001	-0.00034	0.00162	26.261087	26.261617	25.969847	25.970377	16
-0.014357	0.8110	17	57.14342	57.143066	-0.00035	-0.00019	0.00015	27.800940	27.799700	27.495343	27.494103	17
-0.019105	0.6969	18	60.22495	60.224402	-0.00055	-0.00011	0.00008	29.342368	29.342126	29.017666	29.017424	18
-0.016065	0.7910	19	63.30532	63.304661	-0.00066	-0.00021	-0.00010	30.882205	30.882034	30.541438	30.541267	19
-0.017491	0.8077	20	66.38449	66.383618	-0.00087	-0.00027	-0.00005	32.421707	32.422456	32.063449	32.064198	20
-0.017211	0.9074	21	69.46238	69.461241	-0.00114	-0.00046	-0.00020	33.960468	33.961911	33.584999	33.586442	21
-0.018844	0.8241	22	72.53894	72.537337	-0.00160	0.00022	0.00069	35.500122	35.500773	35.105809	35.106460	22
-0.014536		23	75.61411	75.612730	-0.00138	-0.00052	-0.00074	37.037031	37.037215	36.628182	36.628366	23
-0.020506	0.7915	24	78.68783	78.685932	-0.00190	-0.00049	0.00002	38.575777	38.575699	38.146422	38.146344	24
-0.012297	0.8822	25	81.76004	81.757648	-0.00239	-0.00053	-0.00004	40.109211	40.110155	39.667559	39.668503	25
-0.022475	0.8608	26	84.83069	84.827766	-0.00292	-0.00027	0.00026	41.646296	41.648437	41.182169	41.184310	26
-1001.102890	0.9177	27	87.89970	87.896507	-0.00319	-0.00053	-0.00026	##########	43.181470	42.701832	-958.385547	27
1001.567017		28	90.96704	90.963314	-0.00373	-0.00044	0.00010	##########	-956.372342	##########	-956.372342	28
0.000000		29	94.03262	94.028457	-0.00416	-0.00102	-0.00058	##########	-954.342761	##########	-954.342761	29
0.000000		30	97.09641	97.091228	-0.00518	-0.00041	0.00060					30
0.000000		31	100.15833	100.152733	-0.00560	-0.00060	-0.00018					31
		32	103.21833	103.212133	-0.00620	-0.00075	-0.00015					32
		33	106.27634	106.269391	-0.00695	-0.00227	-0.00152					33
		34	109.33232	109.323101	-0.00922	939.68720	939.68947					34
		35	112.38619	##########	939.67798	-1055.11589	-1994.80309					35
		36	115.43791	0.000000	-115.43791	-3.04950	1052.06639					36
			118.48741		-118.48741							
			121.53463									

O-18 Methanol K=2 E1 n=0 (012)													
	R Branch					P Branch	[Series Gamma]				Q Branch		
J	R(J)	Δ1	Δ2	Int.	J	P(J)	Δ1	Δ2	Int.	J	Q(J)	Δ1	Δ2
	1008.189323					1008.186296					1008.190141		
2	1012.728677	1.479650		0.6821	2					2	1008.13929	-0.050852	
3	1014.208327	1.462916	-0.016734	0.5174	3	1003.498730	-1.597146		0.5883	3	1008.08844	-0.066690	-0.015838
4	1015.671243	1.446289	-0.016627	0.4231	4	1001.901584	-1.614458	-0.017312	0.5282	4	1008.02175	-0.084697	-0.018007
5	1017.117532	1.428869	-0.017420	0.3400	5	1000.287126	-1.631490	-0.017032	0.4200	5	1007.93705	-0.097917	-0.013220
6	1018.546401	1.413950	-0.014919	0.1302	6	998.655636	-1.649098	-0.017608	0.2480	6	1007.83913	-0.120605	-0.022688
7	1019.960351	1.395882	-0.018068	0.1987	7	997.006538	-1.665974	-0.016876	0.2180	7	1007.71853	-0.136110	-0.015505
8	1021.356233	1.379451	-0.016431	0.2454	8	995.340564	-1.682919	-0.016945	0.2409	8	1007.58242	##########	-1007.446308
9	1022.735684	1.362085	-0.017366	0.0882	9	993.657645	-1.701253	-0.018334	0.2496	9		0.000000	1007.582418
10	1024.097769	1.345053	-0.017032	0.2189	10	991.956392	-1.716451	-0.015198	0.0464	10		0.000000	0.000000
11	1025.442822	1.327453	-0.017600	0.1872	11	990.239941	-1.734684	-0.018233	0.0277	11		0.000000	0.000000
12	1026.770275	1.308557	-0.018896	0.0695	12	988.505257	-1.751169	-0.016485	0.2148	12		0.000000	0.000000
13	1028.078832	1.290700	-0.017857	0.0828	13	986.754088	-1.767693	-0.016524	0.0463	13		0.000000	0.000000
14	1029.369532	1.272935	-0.017765	0.0877	14	984.986395	-1.783625	-0.015932	0.2232	14		0.000000	0.000000
15	1030.642467	1.252566	-0.020369	0.0708	15	983.202770	-1.799339	-0.015714	0.2530	15		0.000000	0.000000
16	1031.895033	1.233305	-0.019261	0.2628	16	981.403431	-1.814350	-0.015011	0.2587	16		0.000000	0.000000
17	1033.128338	1.213497	-0.019808	0.2992	17	979.589081	-1.829549	-0.015199	0.2170	17		0.000000	0.000000
18	1034.341835	1.193768	-0.019729	0.3198	18	977.759532	-1.843984	-0.014435	0.3113	18		0.000000	0.000000
19	1035.535603	1.174100	-0.019668	0.3549	19	975.915548	-1.858902	-0.014918	0.3279	19		0.000000	0.000000
20	1036.709703	1.154668	-0.019432	0.3923	20	974.056646	-1.873063	-0.014161	0.1200	20		0.000000	0.000000
21	1037.864371	1.135671	-0.018997	0.4267	21	972.183583	-1.887544	-0.014481	0.2725	21		0.000000	0.000000
22	1039.000042	1.116612	-0.019059	0.4796	22	970.296039	-1.902852	-0.015308	0.4711	22		0.000000	0.000000
23	1040.116654	1.098738	-0.017874	0.3097	23	968.393187	-1.918215	-0.015363	0.4856	23		0.000000	0.000000
24	1041.215392	1.080896	-0.017842	0.5619	24	966.474972	-1.933472	-0.015257	0.5544	24		0.000000	0.000000
25	1042.296288	1.061058	-0.019838	0.3985	25	964.541500	-1.949580	-0.016108	0.3455	25		0.000000	0.000000
26	1043.357346	1.043730	-0.017328	0.6552	26	962.591920	-1.965160	-0.015580	0.6427	26		0.000000	0.000000
27	1044.401076	1.025638	-0.018092	0.7022	27	960.626760	-1.980557	-0.015397	0.6741	27		0.000000	0.000000
28	1045.426714	1.007483	-0.018155	0.7428	28	958.646203	-1.997145	-0.016588	0.6780	28		0.000000	0.000000
29	1046.434197	0.989002	-0.018481	0.7762	29	956.649058	-2.012597	-0.015452	0.7729	29		0.000000	0.000000
30	1047.423199	0.971565	-0.017437	0.7267	30	954.636461	-2.028286	-0.015689	0.8064	30		0.000000	0.000000
31	1048.394764	0.953006	-0.018559	0.8247	31	952.608175	-2.043981	-0.015695	0.8456	31		0.000000	0.000000
32	1049.347770	0.935771	-0.017235	0.8572	32	950.564194	-2.059601	-0.015620	0.8582	32			
33	1050.283541	0.917274	-0.018497	0.8760	33	948.504593	-2.075142	-0.015541	0.8899				
34	1051.200815	0.899696	-0.017578	0.9085	34	946.429451	-2.090973	-0.015831	0.8930				
35	1052.100511	0.882884	-0.016812	0.9321	35	944.338478	-2.107310	-0.016337	0.9296				
36	1052.983395	0.865665	-0.017219	0.9373	36	942.231168	-2.123690	-0.016380	0.8946				
37	1053.849060	0.846076	-0.019589	0.9403	37	940.107478	-2.142535	-0.018845	0.9500				
38	1054.695136	0.824772	-0.021304	0.9677	38	937.964943	-2.163375	-0.020840	0.9604				
39	1055.519908	##########	-1056.344680	0.9642	39	935.801568	-2.183429	-0.020054	0.9707				
					40	933.618139	-933.618139	-931.434710	0.9724				

		Calculated	Observed						Ground State Vco=0		Excited State Vco=1		
		R-P Diff	R-P Diff	R-P Diff	Δ1(R-P)	Δ2(R-P)	R-P Diff	a-Type Freq	R(J) a-Type Frequencies		R(J) a-Type Frequencies		
Int.	J	R(J)-P(J+2)	R(J)-P(J+2)	Obs-Calc			MW Obsvns	Microwave	R(J)-Q(J+1)	Q(J)-P(J+1)	R(J)-Q(J)	Q(J+1)-P(J+1)	J
0.4413	2	10.82711	10.827093	-0.00002	-0.00001		10.827109	139106.25	4.640240	4.640559	4.589388	4.589707	2
0.5613	3	13.92123	13.921201	-0.00003	-0.00020	-0.00019		185482.32	6.186580	6.186853	6.119890	6.120163	3
0.5904	4	17.01584	17.015607	-0.00023	0.00018	0.00038			7.734193	7.734621	7.649496	7.649924	4
0.672	5	20.11105	20.110994	-0.00006	-0.00108	-0.00125			9.278399	9.281414	9.180482	9.183497	5
0.0336	6	23.20697	23.205837	-0.00113	0.00012	0.00120			10.827873	10.832595	10.707268	10.711990	6
0.1255	7	26.30372	26.302706	-0.00101	-0.00055	-0.00066			12.377933	12.377964	12.241823	12.241854	7
0.1673	8	29.40140	29.399841	-0.00156	-0.00281	-0.00226			##########	13.924773	13.773815	-993.657645	8
	9	32.50011	32.495743	-0.00437	-0.00310	-0.00029			##########	-991.956392	##########	-991.956392	9
	10	35.59998	35.592512	-0.00747	-0.00491	-0.00181			##########	-990.239941	##########	-990.239941	10
	11	38.70111	38.688734	-0.01238	-0.00735	-0.00245			##########	-988.505257	##########	-988.505257	11
	12	41.80361	41.783880	-0.01973	-0.01179	-0.00443			##########	-986.754088	##########	-986.754088	12
	13	44.90758	44.876062	-0.03152	-0.01553	-0.00374			##########	-984.986395	##########	-984.986395	13
	14	48.01315	47.966101	-0.04705	-0.01998	-0.00444			##########	-983.202770	##########	-983.202770	14
	15	51.12041	51.053386	-0.06702	-0.02695	-0.00698			##########	-981.403431	##########	-981.403431	15
	16	54.22948	54.135501	-0.09398	-0.03370	-0.00675			##########	-979.589081	##########	-979.589081	16
	17	57.34047	57.212790	-0.12768	-0.04061	-0.00691			##########	-977.759532	##########	-977.759532	17
	18	60.45348	60.285189	-0.16829	-0.04832	-0.00771			##########	-975.915548	##########	-975.915548	18
	19	63.56863	63.352020	-0.21661	-0.05576	-0.00744			##########	-974.056646	##########	-974.056646	19
	20	66.68603	66.413664	-0.27237	-0.06223	-0.00647			##########	-972.183583	##########	-972.183583	20
	21	69.80578	69.471184	-0.33460	-0.06832	-0.00609			##########	-970.296039	##########	-970.296039	21
	22	72.92799	72.525070	-0.40292	-0.07471	-0.00638			##########	-968.393187	##########	-968.393187	22
	23	76.05278	75.575154	-0.47763	-0.07916	-0.00446			##########	-966.474972	##########	-966.474972	23
	24	79.18026	78.623472	-0.55679	-0.08420	-0.00504			##########	-964.541500	##########	-964.541500	24
	25	82.31052	81.669528	-0.64099	-0.09156	-0.00735			##########	-962.591920	##########	-962.591920	25
	26	85.44369	84.711143	-0.73255	-0.09531	-0.00376			##########	-960.626760	##########	-960.626760	26
	27	88.57988	87.752018	-0.82786	-0.10107	-0.00575			##########	-958.646203	##########	-958.646203	27
	28	91.71918	90.790253	-0.92893	-0.10677	-0.00571			##########	-956.649058	##########	-956.649058	28
	29	94.86172	93.826022	-1.03570	-0.11289	-0.00612			##########	-954.636461	##########	-954.636461	29
	30	98.00759	96.859005	-1.14858	-0.11816	-0.00528							30
	31	101.15692	99.890171	-1.26675	-0.12474	-0.00658							31
	32	104.30981	102.918319	-1.39149	-0.12982	-0.00507							32
	33	107.46637	105.945063	-1.52131	-0.13576	-0.00594							33
	34	110.62671	108.969647	-1.65706	-0.14083	-0.00508							34
	35	113.79093	111.993033	-1.79790	-0.14281	-0.00198							35
	36	116.95916	115.018452	-1.94071	-0.14329	-0.00048							36
	37	120.13149	118.047492	-2.08400	-0.14705	-0.00376							
	38	123.30804	121.076997	-2.23104	1057.75095	1057.89800							
	39		##########	1055.51991	-1055.51991	-2113.27086							
	40		0.000000	0.00000	0.00000	1055.51991							

O-18 Methanol K=4 E2 n=0 (014)														
	R Branch	[Series N]					P Branch	eries H - K - Ka]					Q Branch	
J	R(J)	Δ1	Δ2	Int.	C	J	P(J)	Δ1	Δ2	Int.	C	J	Q(J)	Δ1
	1008.113017						1008.176121						1008.174702	
4	1015.648597	1.447155		0.3460	*	4						4	1008.005090	-0.084806
5	1017.095752	1.427168	-0.019987	0.5485	*	5	1000.276801	-1.630585		0.2988	*	5	1007.920284	-0.101759
6	1018.522920	1.409584	-0.017584	0.4119	*	6	998.646216	-1.647492	-0.016907	0.1903	*	6	1007.818525	-0.118634
7	1019.932504	1.391952	-0.017632	0.2722	*	7	996.998724	-1.664235	-0.016743	0.1306	*	7	1007.699891	-0.132757
8	1021.324456	1.374249	-0.017703	0.1698	*	8	995.334489	-1.681141	-0.016906	0.0994	*	8	1007.567134	-0.155162
9	1022.698705	1.357702	-0.016547	0.0723	*	9	993.653348	-1.697948	-0.016807	0.0604	*	9	1007.411972	-0.170469
10	1024.056407	1.340562	-0.017140	0.2884	*	10	991.955400	-1.714700	-0.016752	0.0464G*	*	10	1007.241503	-0.187196
11	1025.396969	1.322360	-0.018202	0.1991	*	11	990.240700	-1.731300	-0.016600	0.0277G*	*	11	1007.054307	-0.205936
12	1026.719329	1.304924	-0.017436	0.3144		12	988.509400	-1.747654	-0.016354	0.045G*	*	12	1006.848371	-0.218139
13	1028.024253	1.287283	-0.017641	0.3149		13	986.761746	-1.763997	-0.016343	0.0381	*	13	1006.630232	-0.238408
14	1029.311536	1.269606	-0.017677	0.3329		14	984.997749	-1.780560	-0.016563	0.0565	*	14	1006.391824	-0.253340
15	1030.581142	1.251833	-0.017773	0.3405		15	983.217189	-1.797288	-0.016728	0.0582	*	15	1006.138484	-0.273796
16	1031.832975	1.234022	-0.017811	0.3576		16	981.419901	-1.813758	-0.016470	0.0829	*	16	1005.864688	-0.284503
17	1033.066997	1.216133	-0.017889	0.3850		17	979.606143	-1.830143	-0.016385	0.1334	*	17	1005.580185	-0.308396
18	1034.283130	1.198228	-0.017905	0.4091		18	977.776000	-1.846700	-0.016557	0.1372G*	*	18	1005.271789	-0.326457
19	1035.481358	1.180184	-0.018044	0.3953		19	975.929300	-1.863204	-0.016504	0.2907G*	*	19	1004.945332	##########
20	1036.661542	1.160750	-0.019434	0.4731		20	974.066096	-1.879596	-0.016392	0.3584	*	20		0.000000
21	1037.822292	1.145293	-0.015457	0.2568	*	21	972.186500	-1.895881	-0.016285	0.2725G*	*	21		0.000000
22	1038.967585	1.127156	-0.018137	0.2042	*	22	970.290619	-1.912046	-0.016165	0.4622	*	22		0.000000
23	1040.094741	1.106599	-0.020557	0.3507	*	23	968.378573	-1.928056	-0.016010	0.5012	*	23		0.000000
24	1041.201340	1.089568	-0.017031	0.5979		24	966.450517	-1.944370	-0.016314	0.4899	*	24		0.000000
25	1042.290908	1.070649	-0.018919	0.5838		25	964.506147	-1.960189	-0.015819	0.4667	*	25		0.000000
26	1043.361557	1.052370	-0.018279	0.5843		26	962.545958	-1.978511	-0.018322	0.3594	*	26		0.000000
27	1044.413927	1.033998	-0.018372	0.6591		27	960.567447	-1.994162	-0.015651	0.7405		27		0.000000
28	1045.447925	1.015625	-0.018373	0.6785		28	958.573285	-2.010581	-0.016419	0.7813		28		0.000000
29	1046.463550	0.996488	-0.019137	0.7447		29	956.562704	-2.026844	-0.016263	0.8129		29		0.000000
30	1047.460038	0.979098	-0.017390	0.7314	*	30	954.535860	-2.044932	-0.018088	0.8325		30		0.000000
31	1048.439136	0.959540	-0.019558	0.8676		31	952.490928	-2.058485	-0.013553	0.7670	*	31		0.000000
32	1049.398676	0.940825	-0.018715	0.8664		32	950.432443	-2.075139	-0.016654	0.8194	*	32		
33	1050.339501	0.922093	-0.018732	0.9076		33	948.357304	-2.093390	-0.018251	0.8693	*	33		
34	1051.261594	0.903424	-0.018669	0.8786		34	946.263914	-2.108554	-0.015164	0.8755	*	34		
35	1052.165018	0.886611	-0.016813	0.8738		35	944.155360	-2.126692	-0.018138	0.8895		35		
36	1053.051629	0.861891	-0.024720	0.8664	*	36	942.028668	-2.139677	-0.012985	0.9367	Bd	36		
37	1053.913520	0.844938	-0.016953	0.9162		37	939.888991	-2.157963	-0.018286	0.9248	HS			
38	1054.758458	0.826783	-0.018155	0.8991	*	38	937.731028	-937.731028	-935.573065	0.9625				
39	1055.585241	##########	-1056.412024	0.9045										

			Calculated	Observed				Ground State Vco=0		Excited State Vco=1		
			R-P Diff	R-P Diff	R-P Diff	Δ1(R-P)	Δ2(R-P)	R(J) a-Type Frequencies		R(J) a-Type Frequencies		
Δ2	Int.	J	R(J)-P(J+2)	R(J)-P(J+2)	Obs-Calc			R(J)-Q(J+1)	Q(J)-P(J+1)	R(J)-Q(J)	Q(J+1)-P(J+1)	J
	0.2687	4	17.00807	17.002381	-0.00569	0.00325		7.728313	7.728289	7.643507	7.643483	4
-0.016953	0.3603	5	20.09947	20.097028	-0.00244	0.00049	-0.00275	9.277227	9.274068	9.175468	9.172309	5
-0.016875	0.4427	6	23.19038	23.188431	-0.00195	0.00037	-0.00012	10.823029	10.819801	10.704395	10.701167	6
-0.014123	0.1777	7	26.28073	26.279156	-0.00157	0.00019	-0.00018	12.365370	12.365402	12.232613	12.232645	7
-0.022405	0.4218	8	29.37044	29.369056	-0.00138	-0.00004	-0.00023	13.912484	13.913786	13.757322	13.758624	8
-0.015307	0.2494	9	32.45943	32.458005	-0.00142	0.00079	0.00083	15.457202	15.456572	15.286733	15.286103	9
-0.016727	0.3812	10	35.54764	35.547007	-0.00063	0.00088	0.00008	17.002100	17.000803	16.814904	16.813607	10
-0.018740	0.4201	11	38.63498	38.635223	0.00024	-0.00004	-0.00092	18.548598	18.544907	18.342662	18.338971	11
-0.012203	0.3442	12	41.72138	41.721580	0.00020	0.00010	0.00015	20.089097	20.086625	19.870958	19.868486	12
-0.020269	0.5238	13	44.80676	44.807064	0.00030	0.00027	0.00017	21.632429	21.632483	21.394021	21.394075	13
-0.014932	0.6966	14	47.89106	47.891635	0.00057	0.00023	-0.00004	23.173052	23.174635	22.919712	22.921295	14
-0.020456	0.4956	15	50.97419	50.974999	0.00081	0.00009	-0.00015	24.716454	24.718583	24.442658	24.444787	15
-0.010707	0.5869	16	54.05608	54.056975	0.00090	0.00015	0.00007	26.252790	26.258545	25.968287	25.974042	16
-0.023893	0.4839	17	57.13665	57.137697	0.00105	0.00015	0.00000	27.795208	27.804185	27.486812	27.495789	17
-0.018061	0.7988	18	60.21584	60.217034	0.00119	0.00011	-0.00003	29.337798	29.342489	29.011341	29.016032	18
-1004.618875	0.7850	19	63.29355	63.294858	0.00131	-0.00011	-0.00023	##########	30.879236	30.536026	-974.066096	19
1004.945332		20	66.36973	66.370923	0.00119	-0.00176	-0.00165	##########	-972.186500	##########	-972.186500	20
0.000000		21	69.44429	69.443719	-0.00057	0.00048	0.00224	##########	-970.290619	##########	-970.290619	21
0.000000		22	72.51716	72.517068	-0.00009	0.00043	-0.00005	##########	-968.378573	##########	-968.378573	22
0.000000		23	75.58826	75.588594	0.00033	-0.00247	-0.00290	##########	-966.450517	##########	-966.450517	23
0.000000		24	78.65752	78.655382	-0.00214	0.00074	0.00321	##########	-964.506147	##########	-964.506147	24
0.000000		25	81.72486	81.723461	-0.00140	-0.00054	-0.00128	##########	-962.545958	##########	-962.545958	25
0.000000		26	84.79021	84.788272	-0.00194	-0.00034	0.00020	##########	-960.567447	##########	-960.567447	26
0.000000		27	87.85350	87.851223	-0.00228	-0.00030	0.00004	##########	-958.573285	##########	-958.573285	27
0.000000		28	90.91464	90.912065	-0.00258	0.00164	0.00193	##########	-956.562704	##########	-956.562704	28
0.000000		29	93.97356	93.972622	-0.00094	-0.00166	-0.00329	##########	-954.535860	##########	-954.535860	29
0.000000		30	97.03019	97.027595	-0.00260	-0.00003	0.00162					30
0.000000		31	100.08446	100.081832	-0.00263	0.00111	0.00114					31
		32	103.13628	103.134762	-0.00152	0.00008	-0.00103					32
		33	106.18558	106.184141	-0.00144	0.00209	0.00201					33
		34	109.23228	109.232926	0.00065	-0.00094	-0.00302					34
		35	112.27632	112.276027	-0.00029	0.00327	0.00421					35
		36	115.31762	115.320601	0.00298	-118.35907	-118.36235					36
		37	118.35609		-118.35609							
		38	121.39167									

O-18 Methanol K=1 E1 n=0 (021)

	R Branch						P Branch						Q Branch	
J	R(J)	Δ1	Δ2	Int.	C	J	P(J)	Δ1	Δ2	Int.	C	J	Q(J)	Δ1
	1008.033234						1008.036168						1008.033553	
1	1011.075882	1.495824		0.6939		1						1	1008.016506	-0.034093
2	1012.571706	1.478824	-0.017000	0.5509		2	1004.923708	-1.580911		0.6406		2	1007.982413	-0.050268
3	1014.050530	1.461824	-0.017000	0.4331		3	1003.342797	-1.597365	-0.016454	0.5345		3	1007.932145	-0.068336
4	1015.512354	1.444894	-0.016930	0.3617		4	1001.745432	-1.614232	-0.016867	0.4427		4	1007.863809	##########
5	1016.957248	1.427893	-0.017001	0.3134		5	1000.131200	-1.631100	-0.016868	0.3579		5		0.000000
6	1018.385141	1.410832	-0.017061	0.2665		6	998.500100	-1.647900	-0.016800	0.2961		6		0.000000
7	1019.795973	1.393727	-0.017105	0.2503		7	996.852200	-1.664600	-0.016700	0.2679G*		7		0.000000
8	1021.189700	1.376800	-0.016927	0.1671G*		8	995.187600	-1.681400	-0.016800	0.0779G*		8		0.000000
9	1022.566500	1.359825	-0.016975	0.0496G*		9	993.506200	-1.698200	-0.016800	0.1907G*		9		0.000000
10	1023.926325	1.343143	-0.016682	0.0681		10	991.808000	-1.714884	-0.016684	0.2196		10		0.000000
11	1025.269468	1.326127	-0.017016	0.0644		11	990.093116	-1.731408	-0.016524	0.2084		11		0.000000
12	1026.595595	1.308970	-0.017157	0.0788		12	988.361708	-1.747925	-0.016517	0.2159		12		0.000000
13	1027.904565	1.291971	-0.016999	0.1031		13	986.613783	-1.764598	-0.016673	0.2095		13		0.000000
14	1029.196536	1.273933	-0.018038	0.1439		14	984.849185	-1.780904	-0.016306	0.2291		14		0.000000
15	1030.470469	1.256031	-0.017902	0.1820		15	983.068281	-1.797241	-0.016337	0.2454		15		0.000000
16	1031.726500	1.239200	-0.016831	0.1076G*		16	981.271040	-1.813461	-0.016220	0.2696		16		0.000000
17	1032.965700	1.222385	-0.016815	0.1035G*		17	979.457579	-1.829564	-0.016103	0.2887		17		0.000000
18	1034.188085	1.204592	-0.017793	0.2876		18	977.628015	-1.845668	-0.016104	0.3213		18		0.000000
19	1035.392677	1.186219	-0.018373	0.3379		19	975.782347	-1.861530	-0.015862	0.3204		19		0.000000
20	1036.578896	1.167800	-0.018419	0.3832		20	973.920817	-1.877453	-0.015923	0.3710		20		0.000000
21	1037.746696	1.149676	-0.018124	0.3479		21	972.043364	-1.893199	-0.015746	0.4183		21		0.000000
22	1038.896372	1.130867	-0.018809	0.4802		22	970.150165	-1.908903	-0.015704	0.4646		22		0.000000
23	1040.027239	1.112027	-0.018840	0.5193		23	968.241262	-1.924376	-0.015473	0.5017		23		0.000000
24	1041.139266	1.092687	-0.019340	0.5508		24	966.316886	-1.939886	-0.015510	0.5508		24		0.000000
25	1042.231953	1.073581	-0.019106	0.5465		25	964.377000	-1.955272	-0.015386	0.5979		25		0.000000
26	1043.305534	1.053899	-0.019682	0.6369		26	962.421728	-1.970474	-0.015202	0.6333		26		0.000000
27	1044.359433	1.034559	-0.019340	0.6973		27	960.451254	-1.985713	-0.015239	0.6781		27		0.000000
28	1045.393992	1.014108	-0.020451	0.6003		28	958.465541	-2.000689	-0.014976	0.7309		28		0.000000
29	1046.408100	0.993991	-0.020117	.7099G*Bd		29	956.464852	-2.015798	-0.015109	0.7690		29		0.000000
30	1047.402091	0.973661	-0.020330	0.7569		30	954.449054	-2.030622	-0.014824	0.7978		30		0.000000
31	1048.375752	0.953239	-0.020422	0.8431		31	952.418432	-2.045560	-0.014938	0.8386		31		0.000000
32	1049.328991	0.932871	-0.020368	0.8242		32	950.372872	-2.060259	-0.014699	0.8594		32		
33	1050.261862	0.911737	-0.021134	0.8991		33	948.312613	-2.074613	-0.014354	0.8858				
34	1051.173599	0.890573	-0.021164	0.8915		34	946.238000	-2.089525	-0.014912	G				
35	1052.064172	0.868550	-0.022023	0.8951		35	944.148475	-2.104402	-0.014877	0.9080				
36	1052.932722	0.847979	-0.020571	0.9136		36	942.044073	-2.120875	-0.016473	0.9127				
37	1053.780701	0.826253	-0.021726	0.8716		37	939.923198	-939.923198	-937.802323	0.9563				
38	1054.606954	##########	-1055.433207	0.9467		38		0.000000	939.923198					

			Calculated							Ground State Vco=0		Excited S
			R-P Diff	R-P Diff	R-P Diff	Δ1(R-P)	Δ2(R-P)	R-P Diff	a-Type Freq	R(J) a-Type Frequencies		R(J) a-Type
Δ2	Int.	J	R(J)-P(J+2)	R(J)-P(J+2)	Obs-Calc			MW Obsvns	Microwave	R(J)-Q(J+1)	Q(J)-P(J+1)	R(J)-Q(J)
	0.6575	1	7.73314	7.733085	-0.00006	0.00004		7.733139	92733.95	3.093469	3.092798	3.059376
-0.016175	0.7641	2	10.82629	10.826274	-0.00002	0.00001	-0.00003	10.826287	139099.72	4.639561	4.639616	4.589293
-0.018068	0.8039	3	13.91934	13.919330	-0.00001	0.00000	0.00000		185464.20	6.186721	6.186713	6.118385
-1007.795473	0.7487	4	17.01226	17.012254	-0.00001	0.00004	0.00004		x	##########	7.732609	7.648545
1007.863809		5	20.10501	20.105048	0.00004	-0.00008	-0.00012			##########	-998.500100	##########
0.000000		6	23.19758	23.197541	-0.00004	-0.00012	-0.00004			##########	-996.852200	##########
0.000000		7	26.28993	26.289773	-0.00016	-0.00016	-0.00004			##########	-995.187600	##########
0.000000		8	29.38202	29.381700	-0.00032	-0.00014	0.00003			##########	-993.506200	##########
0.000000		9	32.47384	32.473384	-0.00046	-0.00028	-0.00014			##########	-991.808000	##########
0.000000		10	35.56535	35.564617	-0.00073	-0.00010	0.00017			##########	-990.093116	##########
0.000000		11	38.65652	38.655685	-0.00084	-0.00008	0.00002			##########	-988.361708	##########
0.000000		12	41.74733	41.746410	-0.00092	-0.00054	-0.00045			##########	-986.613783	##########
0.000000		13	44.83774	44.836284	-0.00146	-0.00077	-0.00023			##########	-984.849185	##########
0.000000		14	47.92772	47.925496	-0.00222	-0.00214	-0.00137			##########	-983.068281	##########
0.000000		15	51.01725	51.012890	-0.00436	-0.00346	-0.00132			##########	-981.271040	##########
0.000000		16	54.10630	54.098485	-0.00762	-0.00366	-0.00021			##########	-979.457579	##########
0.000000		17	57.19483	57.183353	-0.01148	-0.00408	-0.00041			##########	-977.628015	##########
0.000000		18	60.28282	60.267268	-0.01555	-0.00537	-0.00130			##########	-975.782347	##########
0.000000		19	63.37024	63.349313	-0.02093	-0.00740	-0.00203			##########	-973.920817	##########
0.000000		20	66.45706	66.428731	-0.02833	-0.00949	-0.00208			##########	-972.043364	##########
0.000000		21	69.54325	69.505434	-0.03782	-0.01147	-0.00198			##########	-970.150165	##########
0.000000		22	72.62877	72.579486	-0.04928	-0.01409	-0.00262			##########	-968.241262	##########
0.000000		23	75.71361	75.650239	-0.06337	-0.01682	-0.00273			##########	-966.316886	##########
0.000000		24	78.79773	78.717538	-0.08019	-0.02021	-0.00339			##########	-964.377000	##########
0.000000		25	81.88110	81.780699	-0.10040	-0.02330	-0.00309			##########	-962.421728	##########
0.000000		26	84.96369	84.839993	-0.12370	-0.02720	-0.00391			##########	-960.451254	##########
0.000000		27	88.04548	87.894581	-0.15090	-0.03059	-0.00339			##########	-958.465541	##########
0.000000		28	91.12643	90.944938	-0.18149	-0.03536	-0.00477			##########	-956.464852	##########
0.000000		29	94.20652	93.989668	-0.21685	-0.03964	-0.00428			##########	-954.449054	##########
0.000000		30	97.28571	97.029219	-0.25649	-0.04435	-0.00471			##########	-952.418432	##########
0.000000		31	100.36398	100.063139	-0.30084	-0.04946	-0.00511			##########	-950.372872	##########
		32	103.44129	103.090991	-0.35030	-0.05393	-0.00448			##########	-948.312613	##########
		33	106.51762	106.113387	-0.40423	-0.05918	-0.00525			##########	-946.238000	##########
		34	109.59294	109.129526	-0.46341	-0.06283	-0.00365			##########	-944.148475	##########
		35	112.66722	112.140974	-0.52625	1053.45897	1053.52180			##########	-942.044073	##########
		36		##########	1052.93272	-1052.93272	-2106.39169			##########	-939.923198	##########
										##########	0.000000	##########
										##########	0.000000	##########
										0.000000	0.000000	0.000000

O-18 Methanol K=2 E2 n=0 (032)

	R Branch						P Branch						Q Branch		
J	R(J)	Δ1	Δ2	Int.	C	J	P(J)	Δ1	Δ2	Int.	C	J	Q(J)	Δ1	Δ2
	1008.151179						1008.137709						1008.153372		
2	1012.694349	1.479502		0.6802		2						2	1008.105281	-0.048091	
3	1014.173851	1.462058	-0.017444	0.2501	*	3	1003.465377	-1.596452		0.6471		3	1008.057190	-0.070403	-0.022312
4	1015.635909	1.445728	-0.016330	0.4248		4	1001.868925	-1.615956	-0.019504	0.3553	*	4	1007.986787	-0.082598	-0.012195
5	1017.081637	1.429048	-0.016680	0.3478		5	1000.252969	-1.632012	-0.016056	0.4256		5	1007.904189	-0.102586	-0.019988
6	1018.510685	1.412983	-0.016065	0.2866		6	998.620957	-1.649433	-0.017421	0.3535		6	1007.801603	##########	-1007.699017
7	1019.923668	1.395368	-0.017615	0.1185	*	7	996.971524	-1.666512	-0.017079	0.3026		7		0.000000	1007.801603
8	1021.319036	1.379669	-0.015699	0.2363		8	995.305012	-1.684182	-0.017670	0.2614		8		0.000000	0.000000
9	1022.698705	1.363083	-0.016586	0.0723	*	9	993.620830	-1.701682	-0.017500	0.2506		9		0.000000	0.000000
10	1024.061788	1.347346	-0.015737	0.1815		10	991.919148	-1.719360	-0.017678	0.2288		10		0.000000	0.000000
11	1025.409134	1.330158	-0.017188	0.0938		11	990.199788	-1.737226	-0.017866	0.2308		11		0.000000	0.000000
12	1026.739292	1.314563	-0.015595	0.2139		12	988.462562	-1.755193	-0.017967	0.2224		12		0.000000	0.000000
13	1028.053855	1.298817	-0.015746	0.1384		13	986.707369	-1.773402	-0.018209	0.2390		13		0.000000	0.000000
14	1029.352672	1.282870	-0.015947	0.2485		14	984.933967	-1.791322	-0.017920	0.2410		14		0.000000	0.000000
15	1030.635542	1.267305	-0.015565	0.2379		15	983.142645	-1.810763	-0.019441	0.1342	*	15		0.000000	0.000000
16	1031.902847	1.251490	-0.015815	0.1624	*	16	981.331882	-1.829869	-0.019106	0.2692		16		0.000000	0.000000
17	1033.154337	1.235488	-0.016002	0.2999		17	979.502013	-1.846853	-0.016984	0.1887	*	17		0.000000	0.000000
18	1034.389825	1.218894	-0.016594	0.3356		18	977.655160	-1.867292	-0.020439	0.3176		18		0.000000	0.000000
19	1035.608719	1.202502	-0.016392	0.3380		19	975.787868	-1.883646	-0.016354	0.2184	*	19		0.000000	0.000000
20	1036.811221	1.188106	-0.014396	0.1882		20	973.904222	-1.902470	-0.018824	0.3902		20		0.000000	0.000000
21	1037.999327	1.164836	-0.023270	0.2987	*	21	972.001752	-1.920258	-0.017788	0.2023	*	21		0.000000	0.000000
22	1039.164163	1.149053	-0.015783	0.4879		22	970.081494	-1.937071	-0.016813	0.4705		22		0.000000	0.000000
23	1040.313216	1.130149	-0.018904	0.5029		23	968.144423	-1.953494	-0.016423	0.5199		23		0.000000	0.000000
24	1041.443365	1.110826	-0.019323	0.5749		24	966.190929	-1.969558	-0.016064	0.5627		24		0.000000	0.000000
25	1042.554191	1.091705	-0.019121	0.5929		25	964.221371	-1.985100	-0.015542	0.6058		25		0.000000	0.000000
26	1043.645896	1.071866	-0.019839	0.6612		26	962.236271	-2.000556	-0.015456	0.6449		26		0.000000	0.000000
27	1044.717762	1.052136	-0.019730	0.7210		27	960.235715	-2.015752	-0.015196	0.6959		27		0.000000	0.000000
28	1045.769898	1.032282	-0.019854	0.7490		28	958.219963	-2.030879	-0.015127	0.7364		28		0.000000	0.000000
29	1046.802180	1.012428	-0.019854	0.7817		29	956.189084	-2.045907	-0.015028	0.7651	L	29		0.000000	0.000000
30	1047.814608	0.992324	-0.020104	0.8109		30	954.143177	-2.060747	-0.014840	0.8139		30		0.000000	0.000000
31	1048.806932	0.972391	-0.019933	0.8569		31	952.082430	-2.076234	-0.015487	0.7946		31		0.000000	0.000000
32	1049.779323	0.952491	-0.019900	0.8705		32	950.006196	-2.090517	-0.014283	0.8504		32			
33	1050.731814	0.929470	-0.023021	0.8958		33	947.915679	-2.105637	-0.015120	0.8765					
34	1051.661284	0.915449	-0.014021	0.8771	HS	34	945.810042	-2.120583	-0.014946	0.9131					
35	1052.576733	0.892070	-0.023379	0.9326		35	943.689459	-2.135434	-0.014851	0.9243					
36	1053.468803	0.872372	-0.019698	0.9372		36	941.554025	-2.150360	-0.014926	0.9378					
37	1054.341175	0.850225	-0.022147	0.9376		37	939.403665	-2.164826	-0.014466	0.9574					
38	1055.191400	0.832803	-0.017422	0.9492		38	937.238839	-937.238839	-935.074013	0.9587					
39	1056.024203	0.808473	-0.024330	0.9595											
40	1056.832676	##########	-1057.641149	0.9522											

		Calculated	Observed						Ground State Vco=0		Excited State Vco=1		
		R-P Diff	R-P Diff	R-P Diff	Δ1(R-P)	Δ2(R-P)	R-P Diff	a-Type Freq	R(J) a-Type Frequencies		R(J) a-Type Frequencies		
Int.	J	R(J)-P(J+2)	R(J)-P(J+2)	Obs-Calc			MW Obsvns	Microwave	R(J)-Q(J+1)	Q(J)-P(J+1)	R(J)-Q(J)	Q(J+1)-P(J+1)	J
0.4879	2	10.82659	10.825424	-0.00117	0.00151		10.826600	139099.72	4.637159	4.639904	4.589068	4.591813	2
0.1424	3	13.92054	13.920882	0.00034	-0.00035	-0.00186		185473.57	6.187064	6.188265	6.116661	6.117862	3
0.6670	4	17.01496	17.014952	-0.00001	0.00016	0.00051			7.731720	7.733818	7.649122	7.651220	4
0.1106	5	20.10996	20.110113	0.00015	-0.00013	-0.00029			9.280034	9.283232	9.177448	9.180646	5
0.3269	6	23.20565	23.205673	0.00002	0.00069	0.00082			##########	10.830079	10.709082	-996.971524	6
	7	26.30213	26.302838	0.00071	-0.00032	-0.00101			##########	-995.305012	##########	-995.305012	7
	8	29.39950	29.399888	0.00039	0.00065	0.00097			##########	-993.620830	##########	-993.620830	8
	9	32.49788	32.498917	0.00104	0.00082	0.00017			##########	-991.919148	##########	-991.919148	9
	10	35.59737	35.599226	0.00186	0.00184	0.00102			##########	-990.199788	##########	-990.199788	10
	11	38.69807	38.701765	0.00370	0.00154	-0.00030			##########	-988.462562	##########	-988.462562	11
	12	41.80009	41.805325	0.00523	0.00245	0.00091			##########	-986.707369	##########	-986.707369	12
	13	44.90353	44.911210	0.00768	0.00460	0.00215			##########	-984.933967	##########	-984.933967	13
	14	48.00851	48.020790	0.01228	0.00613	0.00153			##########	-983.142645	##########	-983.142645	14
	15	51.11512	51.133529	0.01841	0.00580	-0.00033			##########	-981.331882	##########	-981.331882	15
	16	54.22348	54.247687	0.02421	0.00858	0.00278			##########	-979.502013	##########	-979.502013	16
	17	57.33368	57.366469	0.03279	0.00698	-0.00160			##########	-977.655160	##########	-977.655160	17
	18	60.44583	60.485603	0.03977	0.00715	0.00017			##########	-975.787868	##########	-975.787868	18
	19	63.56004	63.606967	0.04693	0.00638	-0.00077			##########	-973.904222	##########	-973.904222	19
	20	66.67642	66.729727	0.05331	0.00653	0.00015			##########	-972.001752	##########	-972.001752	20
	21	69.79507	69.854904	0.05983	-0.00269	-0.00922			##########	-970.081494	##########	-970.081494	21
	22	72.91609	72.973234	0.05714	-0.00489	-0.00220			##########	-968.144423	##########	-968.144423	22
	23	76.03959	76.091845	0.05226	-0.01084	-0.00595			##########	-966.190929	##########	-966.190929	23
	24	79.16568	79.207094	0.04141	-0.01740	-0.00656			##########	-964.221371	##########	-964.221371	24
	25	82.29446	82.318476	0.02402	-0.02411	-0.00671			##########	-962.236271	##########	-962.236271	25
	26	85.42603	85.425933	-0.00010	-0.03173	-0.00762			##########	-960.235715	##########	-960.235715	26
	27	88.56051	88.528678	-0.03183	-0.03945	-0.00771			##########	-958.219963	##########	-958.219963	27
	28	91.69800	91.626721	-0.07128	-0.04757	-0.00812			##########	-956.189084	##########	-956.189084	28
	29	94.83860	94.719750	-0.11885	-0.05516	-0.00759			##########	-954.143177	##########	-954.143177	29
	30	97.98242	97.808412	-0.17401	-0.06431	-0.00915							30
	31	101.12957	100.891253	-0.23832	-0.07255	-0.00824							31
	32	104.28015	103.969281	-0.31087	-0.08104	-0.00846							32
	33	107.43426	107.042355	-0.39191	-0.09285	-0.01181							33
	34	110.59201	110.107259	-0.48475	-0.09570	-0.00285							34
	35	113.75352	113.173068	-0.58045	-0.10845	-0.01275							35
	36	116.91887	116.229964	-0.68891	-119.39927	-119.29082							36
		120.08818		-120.08818									
		123.26156											

O-18 Methanol K=3 E1 n=0 (033)														
	R Branch	[Series F]					P Branch						Q Branch	
J	R(J)	Δ1	Δ2	Int.	C	J	P(J)	Δ1	Δ2	Int.	C	J	Q(J)	Δ1
	1008.206158						1008.213316						1008.214644	
3	1014.229710	1.462003		0.6162		3						3	1008.112596	-0.068032
4	1015.691713	1.444449	-0.017554	0.5462		4	1001.926788	-1.614287		0.6975		4	1008.044564	-0.084899
5	1017.136162	1.427496	-0.016953	0.4468		5	1000.312501	-1.631349	-0.017062	0.5440		5	1007.959665	-0.102001
6	1018.563658	1.410442	-0.017054	0.3660		6	998.681152	-1.648405	-0.017056	0.4484	*	6	1007.857664	-0.117464
7	1019.974100	1.393605	-0.016837	0.3102		7	997.032747	-1.665373	-0.016968	0.3687	*	7	1007.740200	-0.137451
8	1021.367705	1.376207	-0.017398	0.2037		8	995.367374	-1.682076	-0.016703	0.0956	*	8	1007.602749	##########
9	1022.743912	1.359222	-0.016985	0.2728		9	993.685298	-1.699296	-0.017220	0.3004		9		0.000000
10	1024.103134	1.342012	-0.017210	0.2654		10	991.986002	-1.716303	-0.017007	0.2879		10		0.000000
11	1025.445146	1.325129	-0.016883	0.2242		11	990.269699	-1.733405	-0.017102	0.2726		11		0.000000
12	1026.770275	1.308557	-0.016572	0.0695	*	12	988.536294	-1.750498	-0.017093	0.2742		12		0.000000
13	1028.078832	1.290700	-0.017857	0.0828	*	13	986.785796	-1.767079	-0.016581	0.2180		13		0.000000
14	1029.369532	1.272935	-0.017765	0.0877	*	14	985.018717	-1.783678	-0.016599	0.0938	*	14		0.000000
15	1030.642467	1.256699	-0.016236	0.0708	*	15	983.235039	-1.802794	-0.019116	0.0759	*	15		0.000000
16	1031.899166	1.238733	-0.017966	0.2911		16	981.432245	-1.818686	-0.015892	0.3045		16		0.000000
17	1033.137899	1.222231	-0.016502	0.2627	*	17	979.613559	-1.836645	-0.017959	0.3317		17		0.000000
18	1034.360130	1.204529	-0.017702	0.3539		18	977.776914	-1.851688	-0.015043	0.1372	*	18		0.000000
19	1035.564659	1.187170	-0.017359	0.3989		19	975.925226	-1.868580	-0.016892	0.2907	*	19		0.000000
20	1036.751829	1.169750	-0.017420	0.4413		20	974.056646	-1.888378	-0.019798	0.1200	*	20		0.000000
21	1037.921579	1.152249	-0.017501	0.4755		21	972.168268	-1.905005	-0.016627	0.2980	*	21		0.000000
22	1039.073828	1.134502	-0.017747	0.5104		22	970.263263	-1.921537	-0.016532	0.4991		22		0.000000
23	1040.208330	1.117610	-0.016892	0.4420		23	968.341726	-1.938404	-0.016867	0.5254		23		0.000000
24	1041.325940	1.099144	-0.018466	0.5100	*	24	966.403322	-1.955600	-0.017196	0.5768		24		0.000000
25	1042.425084	1.082019	-0.017125	0.6453		25	964.447722	-1.972584	-0.016984	0.6230		25		0.000000
26	1043.507103	1.063241	-0.018778	0.5584		26	962.475138	-1.989646	-0.017062	0.6703		26		0.000000
27	1044.570344	1.045633	-0.017608	0.7311		27	960.485492	-2.006511	-0.016865	0.7088		27		0.000000
28	1045.615977	1.027915	-0.017718	0.7083		28	958.478981	-2.023358	-0.016847	0.7438		28		0.000000
29	1046.643892	1.008887	-0.019028	0.6106	*	29	956.455623	-2.040253	-0.016895	0.7811		29		0.000000
30	1047.652779	0.990702	-0.018185	0.8343		30	954.415370	-2.056766	-0.016513	0.8262		30		0.000000
31	1048.643481	0.971705	-0.018997	0.8538		31	952.358604	-2.073247	-0.016481	0.8490		31		0.000000
32	1049.615186	0.953629	-0.018076	0.8671		32	950.285357	-2.089550	-0.016303	0.8689		32		
33	1050.568815	0.934555	-0.019074	0.8884	*	33	948.195807	-2.105536	-0.015986	0.8999				
34	1051.503370	0.913578	-0.020977	0.8504	*	34	946.090271	-2.121538	-0.016002	0.9098				
35	1052.416948	0.894799	-0.018779	0.8872	*	35	943.968733	-2.137130	-0.015592	0.9090				
36	1053.311747	0.875319	-0.019480	0.9038	*	36	941.831603	-2.151534	-0.014404	0.8999	*			
37	1054.187066	##########	-1055.062385	0.9437		37	939.680069	-939.680069	-937.528535	0.9501				

			Calculated	Observed				Ground State Vco=0		Excited State Vco=1		
			R-P Diff	R-P Diff	R-P Diff	Δ1(R-P)	Δ2(R-P)	R(J) a-Type Frequencies		R(J) a-Type Frequencies		
Δ2	Int.	J	R(J)-P(J+2)	R(J)-P(J+2)	Obs-Calc			R(J)-Q(J+1)	Q(J)-P(J+1)	R(J)-Q(J)	Q(J+1)-P(J+1)	J
	0.3116	3	13.91770	13.917209	-0.00049	0.00056		6.185146	6.185808	6.117114	6.117776	3
-0.016867	0.4350	4	17.01049	17.010561	0.00007	0.00006	-0.00050	7.732048	7.732063	7.647149	7.647164	4
-0.017102	0.5347	5	20.10328	20.103415	0.00014	0.00010	0.00003	9.278498	9.278513	9.176497	9.176512	5
-0.015463	0.3793	6	23.19605	23.196284	0.00023	-0.00023	-0.00033	10.823458	10.824917	10.705994	10.707453	6
-0.019987	0.3913	7	26.28880	26.288802	0.00000	0.00017	0.00040	12.371351	12.372826	12.233900	12.235375	7
-1007.465298	0.7054	8	29.38153	29.381703	0.00017	-0.00020	-0.00037	##########	13.917451	13.764956	-993.685298	8
1007.602749		9	32.47424	32.474213	-0.00003	-0.00005	0.00015	##########	-991.986002	##########	-991.986002	9
0.000000		10	35.56692	35.566840	-0.00008	-0.00014	-0.00009	##########	-990.269699	##########	-990.269699	10
0.000000		11	38.65957	38.659350	-0.00022	-0.00042	-0.00028	##########	-988.536294	##########	-988.536294	11
0.000000		12	41.75220	41.751558	-0.00064	-0.00036	0.00007	##########	-986.785796	##########	-986.785796	12
0.000000		13	44.84479	44.843793	-0.00100	0.00094	0.00130	##########	-985.018717	##########	-985.018717	13
0.000000		14	47.93734	47.937287	-0.00005	-0.00090	-0.00184	##########	-983.235039	##########	-983.235039	14
0.000000		15	51.02986	51.028908	-0.00095	0.00086	0.00176	##########	-981.432245	##########	-981.432245	15
0.000000		16	54.12234	54.122252	-0.00009	-0.00201	-0.00287	##########	-979.613559	##########	-979.613559	16
0.000000		17	57.21477	57.212673	-0.00210	-0.00158	0.00043	##########	-977.776914	##########	-977.776914	17
0.000000		18	60.30716	60.303484	-0.00368	0.00057	0.00215	##########	-975.925226	##########	-975.925226	18
0.000000		19	63.39950	63.396391	-0.00311	-0.00011	-0.00068	##########	-974.056646	##########	-974.056646	19
0.000000		20	66.49179	66.488566	-0.00322	-0.00095	-0.00084	##########	-972.168268	##########	-972.168268	20
0.000000		21	69.58403	69.579853	-0.00418	-0.00154	-0.00058	##########	-970.263263	##########	-970.263263	21
0.000000		22	72.67622	72.670506	-0.00571	-0.00202	-0.00048	##########	-968.341726	##########	-968.341726	22
0.000000		23	75.76834	75.760608	-0.00773	-0.00186	0.00014	##########	-966.403322	##########	-966.403322	23
0.000000		24	78.86041	78.850802	-0.00961	-0.00321	-0.00133	##########	-964.447722	##########	-964.447722	24
0.000000		25	81.95241	81.939592	-0.01282	-0.00342	-0.00021	##########	-962.475138	##########	-962.475138	25
0.000000		26	85.04436	85.028122	-0.01624	-0.00527	-0.00185	##########	-960.485492	##########	-960.485492	26
0.000000		27	88.13623	88.114721	-0.02151	-0.00591	-0.00064	##########	-958.478981	##########	-958.478981	27
0.000000		28	91.22803	91.200607	-0.02742	-0.00705	-0.00113	##########	-956.455623	##########	-956.455623	28
0.000000		29	94.31976	94.285288	-0.03447	-0.00953	-0.00248	##########	-954.415370	##########	-954.415370	29
0.000000		30	97.41142	97.367422	-0.04400	-0.01133	-0.00180	##########	-952.358604	##########	-952.358604	30
0.000000		31	100.50300	100.447674	-0.05533	-0.01426	-0.00293	##########	-950.285357	##########	-950.285357	31
		32	103.59450	103.524915	-0.06959	-0.01625	-0.00199	##########	-948.195807	##########	-948.195807	32
		33	106.68592	106.600082	-0.08584	-0.01966	-0.00340					33
		34	109.77726	109.671767	-0.10549	-0.02614	-0.00648					34
		35	112.86851	112.736879	-0.13163	937.48371	937.50985					35
		36	115.95967	##########	937.35208	-2.21575	-939.69946					36
		37	119.05074	##########	935.13633	-1057.27804	-1055.06229					
		38	122.14171	0.000000	-122.14171	122.14171	1179.41975					
				0.000000	0.00000	0.00000	-122.14171					
					0.00000							

B.2 Assigning process pieces

The following part is abstracted from a file `typescript` which records the MOSAA assigning process for series (035)E2 in this spectrum.

```
-------------------------------------------------------------
** Do select_bottom_line(  , 5178,  , 5177,  , )

choice 1:
The candidate is from down extracting
 SpreadSheet is:
 R,
parm=Cur_Peaks[15].J,  has_J=0
Index    J        wv          delta1      delta2      intens
15.           1027.861745   1.348672                0.383996
16.           1029.210417   1.327538   -0.021134    0.660026
17.           1030.537955   1.309073   -0.018465    0.533268
18.           1031.847028                           0.301236



choice 2:
The candidate is from down extracting
 SpreadSheet is:
 R,
parm=Cur_Peaks[15].J,  has_J=0
Index    J        wv          delta1      delta2      intens
15.           1027.861745   1.348672                0.383996
16.           1029.210417   1.327538   -0.021134    0.660026
17.           1030.537955   1.304082   -0.023456    0.533268
18.           1031.842037                           0.264357

Please pick one (1,  2,  or 0-none of them):
2
                                                  ( part A )
-------------------------------------------------------------

 SpreadSheet is:
 R,
parm=Cur_Peaks[7].J,  has_J=0
Index    J        wv          delta1      delta2      intens
 7.           1016.935647   1.427823                0.752472
 8.           1018.363470   1.407774   -0.020049    0.223020
 9.           1019.771244   1.391835   -0.015939    0.538795
10.           1021.163079   1.374718   -0.017117    0.463053
11.           1022.537797   1.357109   -0.017609    0.391154
12.           1023.894906   1.336639   -0.020470    0.384100
13.           1025.233545   1.321518   -0.015121    0.538079
14.           1026.553063   1.308682   -0.012836    0.189987
15.           1027.861745   1.294771   -0.013911    0.383996
16.           1029.156516   1.280764   -0.014007    0.565841
17.           1030.437280                           0.267685



----4
** Do select_modify_type( )

add line ------- a
modify line ---- m
delete line ---- d
no operation --- n
Add a missed peak into .pkf file --- p
Change CD type --- c
This series is totally wrong, quit --- q
```

```
                                                  ( part B )
-------------------------------------------------------------
** Do select_bottom_line(  , 6076,  , 6075,  , )

choice 1:
The candidate is from down extracting
 SpreadSheet is:
 R,
parm=Cur_Peaks[7].J,  has_J=0
Index    J        wv          delta1      delta2      intens
 7.           1016.935647   1.427823                0.752472
 8.           1018.363470   1.407774   -0.020049    0.223020
 9.           1019.771244   1.391835   -0.015939    0.538795
10.           1021.163079   1.374718   -0.017117    0.463053
11.           1022.537797   1.357109   -0.017609    0.391154
12.           1023.894906   1.339657   -0.017452    0.384100
13.           1025.234563   1.322407   -0.017250    0.388059
14.           1026.556970   1.304775   -0.017632    0.385661
15.           1027.861745   1.287316   -0.017459    0.383996
16.           1029.149061   1.269753   -0.017563    0.391489
17.           1030.418814   1.252379   -0.017374    0.412323
18.           1031.671193   1.234256   -0.018123    0.292232
19.           1032.905449   1.216726   -0.017530    0.437019
20.           1034.122175   1.199070   -0.017656    0.461675
21.           1035.321245   1.181244   -0.017826    0.463786
22.           1036.502489   1.163292   -0.017952    0.495581
23.           1037.665781   1.145341   -0.017951    0.566984
24.           1038.811122   1.128060   -0.017281    0.591718
25.           1039.939182   1.109391   -0.018669    0.358014
26.           1041.048573   1.091782   -0.017609    0.673769
27.           1042.140355                           0.707450


choice 2:
The candidate is from down extracting
 SpreadSheet is:
 R,
parm=Cur_Peaks[7].J,  has_J=0
Index    J        wv          delta1      delta2      intens
 7.           1016.935647   1.427823                0.752472
 8.           1018.363470   1.407774   -0.020049    0.223020
 9.           1019.771244   1.391835   -0.015939    0.538795
10.           1021.163079   1.374718   -0.017117    0.463053
11.           1022.537797   1.357109   -0.017609    0.391154
12.           1023.894906   1.339657   -0.017452    0.384100
13.           1025.234563   1.322407   -0.017250    0.388059
14.           1026.556970   1.304775   -0.017632    0.385661
15.           1027.861745   1.287316   -0.017459    0.383996
16.           1029.149061   1.269753   -0.017563    0.391489
17.           1030.418814   1.252379   -0.017374    0.412323
18.           1031.671193   1.234256   -0.018123    0.292232
19.           1032.905449   1.216726   -0.017530    0.437019
20.           1034.122175   1.199070   -0.017656    0.461675
21.           1035.321245   1.181244   -0.017826    0.463786
22.           1036.502489   1.163292   -0.017952    0.495581
23.           1037.665781   1.145341   -0.017951    0.566984
24.           1038.811122   1.128060   -0.017281    0.591718
```

```
25.          1039.939182   1.109391   -0.018669   0.358014
26.          1041.048573   1.084280   -0.025111   0.673768
27.          1042.132853                          0.624209

                                                 ( part C )
--------------------------------------------------------------
 SpreadSheet is:
 R,
parm=Cur_Peaks[7].J,   has_J=0
Index    J       wv          delta1       delta2       intens
 7.          1016.935647   1.427823                0.752472
 8.          1018.363470   1.407774   -0.020049   0.223020
 9.          1019.771244   1.391835   -0.015939   0.538795
10.          1021.163079   1.374718   -0.017117   0.463053
11.          1022.537797   1.357109   -0.017609   0.391154
12.          1023.894906   1.339657   -0.017452   0.384100
13.          1025.234563   1.322407   -0.017250   0.388059
14.          1026.556970   1.304775   -0.017632   0.385661
15.          1027.861745   1.287316   -0.017459   0.383996
16.          1029.149061   1.269753   -0.017563   0.391489
17.          1030.418814   1.252379   -0.017374   0.412323
18.          1031.671193   1.234256   -0.018123   0.292232
19.          1032.905449   1.216726   -0.017530   0.437019
20.          1034.122175   1.199070   -0.017656   0.461675
21.          1035.321245   1.181244   -0.017826   0.463786
22.          1036.502489   1.163292   -0.017952   0.495581
23.          1037.665781   1.145341   -0.017951   0.566984
24.          1038.811122   1.128060   -0.017281   0.591718
25.          1039.939182   1.109391   -0.018669   0.358014
26.          1041.048573   1.091782   -0.017609   0.673768
27.          1042.140355   1.072958   -0.018824   0.707450
28.          1043.213313   1.055536   -0.017422   0.740337
29.          1044.268849   1.037226   -0.018310   0.758308
30.          1045.306075   1.019244   -0.017982   0.804152
31.          1046.325319   1.000979   -0.018265   0.815091
32.          1047.326298   0.982764   -0.018215   0.856984
33.          1048.309062                          0.876332

                                                 ( part D )
--------------------------------------------------------------

choice 1:
The candidate is from up extracting
 SpreadSheet is:
K=5 n=0 Symm=E2
 P,
parm=Cur_Peaks[16].J,   has_J=1
Index    J       wv          delta1       delta2       intens
16.  16.     984.839562  -1.783680                0.259630
17.  15.     983.055882  -1.799284   -0.015604   0.193820
18.  16.     981.256598  -1.816869   -0.017585   0.134669
19.  17.     979.439729                          0.081400



choice 2:
The candidate is from R branch
 SpreadSheet is:
K=5 n=0 Symm=E2
 P,
```

```
parm=Cur_Peaks[16].J,   has_J=1
Index    J       wv          delta1       delta2       intens
16.  16.     984.836326  -1.780444                0.333168
17.  15.     983.055882  -1.799284   -0.018840   0.193820
18.  16.     981.256598  -1.816869   -0.017585   0.134669
19.  17.     979.439729                          0.081400

                                                 ( part E )
--------------------------------------------------------------

choice 1:
The candidate is from R branch
 SpreadSheet is:
K=5 n=0 Symm=E2
 P,
parm=Cur_Peaks[7].J,   has_J=1
Index    J       wv          delta1       delta2       intens
 7.   5.    1000.124774  -1.638297                0.260442
 8.   6.     998.486477  -1.648139   -0.009842   0.758371
 9.   7.     996.838338  -1.663821   -0.015682   0.189422
10.   8.     995.174517  -1.681219   -0.017398   0.541212
11.   9.     993.493298  -1.697869   -0.016650   0.476969
12.  10.     991.795429  -1.714657   -0.016788   0.426428
13.  11.     990.080772  -1.731541   -0.016884   0.389787
14.  12.     988.349231  -1.748136   -0.016595   0.397904
15.  13.     986.601095  -1.764769   -0.016633   0.390530
16.  14.     984.836326  -1.780444   -0.015675   0.333168
17.  15.     983.055882  -1.799284   -0.018840   0.193820
18.  16.     981.256598  -1.816869   -0.017585   0.134669
19.  17.     979.439729  -1.829323   -0.012454   0.081400
20.  18.     977.610406                          0.451722


choice 2:
The candidate is from down extracting
 SpreadSheet is:
K=5 n=0 Symm=E2
 P,
parm=Cur_Peaks[7].J,   has_J=1
Index    J       wv          delta1       delta2       intens
 7.   5.    1000.124774  -1.638297                0.260442
 8.   6.     998.486477  -1.648139   -0.009842   0.758371
 9.   7.     996.838338  -1.663821   -0.015682   0.189422
10.   8.     995.174517  -1.681219   -0.017398   0.541212
11.   9.     993.493298  -1.697869   -0.016650   0.476969
12.  10.     991.795429  -1.714657   -0.016788   0.426428
13.  11.     990.080772  -1.731541   -0.016884   0.389787
14.  12.     988.349231  -1.748136   -0.016595   0.397904
15.  13.     986.601095  -1.764769   -0.016633   0.390530
16.  14.     984.836326  -1.780444   -0.015675   0.333168
17.  15.     983.055882  -1.799284   -0.018840   0.193820
18.  16.     981.256598  -1.816869   -0.017585   0.134669
19.  17.     979.439729  -1.834049   -0.017180   0.081400
20.  18.     977.605680                          0.326282

                                                 ( part F )
--------------------------------------------------------------
```

```
 SpreadSheet is:
K=5 n=0 Symm=E2
 P,
parm=Cur_Peaks[7|.J,  has_J=1
Index    J         wv          delta1       delta2      intens
 7.    5.   1000.124774  -1.638297                   0.260442
 8.    6.    998.486477  -1.648139   -0.009842   0.758371
 9.    7.    996.838338  -1.663821   -0.015682   0.189422
10.    8.    995.174517  -1.681219   -0.017398   0.541212
11.    9.    993.493298  -1.697869   -0.016650   0.476969
12.   10.    991.795429  -1.714657   -0.016788   0.426428
13.   11.    990.080772  -1.731541   -0.016884   0.389787
14.   12.    988.349231  -1.748136   -0.016595   0.397904
15.   13.    986.601095  -1.764769   -0.016633   0.380530
16.   14.    984.836326  -1.780444   -0.015675   0.333168
17.   15.    983.055882  -1.799284   -0.018840   0.193820
18.   16.    981.256598  -1.816869   -0.017585   0.134669
19.   17.    979.439729  -1.829323   -0.012454   0.081400
20.   18.    977.610406  -1.848023   -0.018700   0.451722
21.   19.    975.762383  -1.864610   -0.016587   0.502319
22.   20.    973.897773  -1.881189   -0.016579   0.526464
23.   21.    972.016584  -1.897713   -0.016524   0.564379
24.   22.    970.118871  -1.914331   -0.016618   0.595595
25.   23.    968.204540  -1.930755   -0.016424   0.637357
26.   24.    966.273785  -1.947333   -0.016578   0.669913
27.   25.    964.326452  -1.963811   -0.016478   0.693673
28.   26.    962.362641  -1.979934   -0.016123   0.734873
29.   27.    960.382707  -1.997160   -0.017226   0.780559
30.   28.    958.385547  -2.013205   -0.016045   0.771466
31.   29.    956.372342  -2.029581   -0.016376   0.830546
32.   30.    954.342761  -2.045899   -0.016318   0.865747
33.   31.    952.296862  -2.061792   -0.015893   0.886320
34.   32.    950.235070  -2.078741   -0.016949   0.786002
35.   33.    948.156329  -2.094354   -0.015613   0.919047
36.   34.    946.061975                            0.931037


                                                    ( part G )
--------------------------------------------------------------
****************************************
4271  1018.363470     0.223020
*****************************************
** Do ask_y_n_ques( Line seems overlapped, adjust it's intensity?, )


Line seems overlapped, adjust it's intensity?
                                                    ( part H )
--------------------------------------------------------------

 SpreadSheet is:
K=5 n=0 Symm=E2
 R,
parm=Cur_Peaks[7].J,  has_J=1
Index    J        wv          delta1       delta2      intens
 7.    5.   1016.935647   1.427823                  0.752472
 8.    6.   1018.363470   1.407774   -0.020049   0.614537
 9.    7.   1019.771244   1.391835   -0.015939   0.538795
10.    8.   1021.163079   1.374718   -0.017117   0.463053
11.    9.   1022.537797   1.357109   -0.017609   0.391154
12.   10.   1023.894906   1.339657   -0.017452   0.384100
13.   11.   1025.234563   1.322407   -0.017250   0.388059
14.   12.   1026.556970   1.304775   -0.017632   0.385661
15.   13.   1027.861745   1.287316   -0.017459   0.383996
16.   14.   1029.149061   1.269753   -0.017563   0.391489
17.   15.   1030.418814   1.252379   -0.017374   0.412323
18.   16.   1031.671193   1.234256   -0.018123   0.292232
19.   17.   1032.905449   1.216726   -0.017530   0.437019
20.   18.   1034.122175   1.199070   -0.017656   0.461675
21.   19.   1035.321245   1.181244   -0.017826   0.463786
22.   20.   1036.502489   1.163292   -0.017952   0.495581
23.   21.   1037.665781   1.145341   -0.017951   0.566984
24.   22.   1038.811122   1.128060   -0.017281   0.591718
25.   23.   1039.939182   1.109391   -0.018669   0.358014
26.   24.   1041.048573   1.091782   -0.017609   0.673768
27.   25.   1042.140355   1.072958   -0.018824   0.707450
28.   26.   1043.213313   1.055536   -0.017422   0.740337
29.   27.   1044.268849   1.037226   -0.018310   0.758308
30.   28.   1045.306075   1.019244   -0.017982   0.804152
31.   29.   1046.325319   1.000979   -0.018265   0.815091
32.   30.   1047.326298   0.982764   -0.018215   0.856984
33.   31.   1048.309062                           0.876332

                                                    ( part I )
--------------------------------------------------------------
The output for this series is in file: series0.output
Do you want to export current information into 'new.ass_pkf'
```

B.3 MOSAA assigned series outputs for input spectrum of $CH_3^{18}OH$ in the 900-1100 cm^{-1} region.

There are 11 series assigned in this testing. The format of the outputs from MOSAA is similar to the one used in the spreadsheet files. Output of each series (if it has a Q branch) is split into two pages manually just for reading purposes.

The outputs show the assigned lines in R, P and Q branches for each series[1]. The left part of the top line '`K=0, n=0 A` ' shows the values of K, n and asymmetry of this series, which is produced by MOSAA. The center part of the top line '`(010)A`' corresponds to (n τ K) asymmetry of the series, which was added manually by the user[2]. A '`c`' in column '`Comm`' of each branch of the series shows if the line is RPQ confirmed.

---

[1] These are the output from the computer, some lines are not correct. Table 6.1 gives the summary of which lines are correct.

[2] As mentioned in section 6.1.1, the τ value can be obtained from the n and K values, this function can be added in MOSAA easily using a lookup table in the future.

K=0 n=0 A (010)A

R_branch						P_branch					
J	wv	delta1	delta2	intens	Comm	J	wv	delta1	delta2	intens	Comm
0.	1009.478034	1.512668		0.753032							
1.	1010.990702	1.495372	-0.017296	0.619716		1.	1006.402789	-1.563911		0.552857	
2.	1012.486074	1.478293	-0.017079	0.473790		2.	1004.838878	-1.580442	-0.016531	0.524612	
3.	1013.964367	1.461013	-0.017280	0.387242		3.	1003.258436	-1.596679	-0.016237	0.475005	
4.	1015.425380	1.443217	-0.017796	0.300434		4.	1001.661757	-1.613218	-0.016539	0.395773	
5.	1016.868597	1.425843	-0.017374	0.267698		5.	1000.048539	-1.629579	-0.016361	0.321836	
6.	1018.294440	1.408141	-0.017702	0.237105		6.	998.418960	-1.645901	-0.016322	0.289601	
7.	1019.702581	1.390439	-0.017702	0.225094		7.	996.773059	-1.662153	-0.016252	0.256161	
8.	1021.093020	1.372526	-0.017913	0.204091		8.	995.110906	-1.678162	-0.016009	0.220218	
9.	1022.465546	1.354544	-0.017982	0.190227		9.	993.432744	-1.694210	-0.016048	0.196990	
10.	1023.820090	1.336475	-0.018069	0.186490		10.	991.738534	-1.710096	-0.015886	0.199382	
11.	1025.156565	1.318298	-0.018177	0.191595		11.	990.028438	-1.725872	-0.015776	0.189345	
12.	1026.474863	1.300135	-0.018163	0.173582		12.	988.302566	-1.741569	-0.015697	0.195080	
13.	1027.774998	1.281724	-0.018411	0.181819		13.	986.560997	-1.757174	-0.015605	0.202004	
14.	1029.056722	1.263382	-0.018342	0.209376		14.	984.803823	-1.772661	-0.015487	0.208210	
15.	1030.320104	1.244706	-0.018676	0.205856		15.	983.031162	-1.788094	-0.015433	0.220821	
16.	1031.564810	1.226364	-0.018342	0.216623		16.	981.243068	-1.803339	-0.015245	0.236574	
17.	1032.791174	1.207633	-0.018731	0.249727		17.	979.439729	-1.818764	-0.015425	0.081400	
18.	1033.998807	1.188964	-0.018669	0.283559		18.	977.620965	-1.833097	-0.014333	0.291503	
19.	1035.187771	1.170591	-0.018373	0.312310		19.	975.787868	-1.849606	-0.016509	0.218430	
20.	1036.358362	1.151221	-0.019370	0.320616		20.	973.938262	-1.863971	-0.014365	0.361043	
21.	1037.509583	1.132707	-0.018514	0.394330		21.	972.074291	-1.878919	-0.014948	0.388937	
22.	1038.642290	1.113961	-0.018746	0.455210		22.	970.195372	-1.894017	-0.015098	0.427641	
23.	1039.756251	1.095120	-0.018841	0.495044		23.	968.301355	-1.908561	-0.014544	0.418080	
24.	1040.851371	1.076342	-0.018778	0.537341		24.	966.392794	-1.923588	-0.015027	0.524686	
25.	1041.927713	1.057517	-0.018825	0.556384		25.	964.469206	-1.937831	-0.014243	0.563720	
26.	1042.985230	1.038646	-0.018871	0.625483		26.	962.531375	-1.953736	-0.015905	0.390847	
27.	1044.023876	1.020085	-0.018561	0.667567		27.	960.577639	-1.967628	-0.013892	0.658607	
28.	1045.043961	1.001401	-0.018684	0.706704		28.	958.610011	-1.983252	-0.015624	0.682300	
29.	1046.045362	0.982436	-0.018965	0.745031		29.	956.626759	-1.997667	-0.014415	0.756327	
30.	1047.027798	0.963892	-0.018544	0.789598		30.	954.629092	-2.012495	-0.014828	0.781900	
31.	1047.991690	0.945035	-0.018857	0.785441		31.	952.616597	-2.027316	-0.014821	0.820027	
32.	1048.936725	0.927162	-0.017873	0.845362		32.	950.589281	-2.042550	-0.015234	0.837584	
33.	1049.863887	0.908072	-0.019090	0.879778		33.	948.546731	-2.056953	-0.014403	0.865546	
34.	1050.771959	0.889325	-0.018747	0.839085		34.	946.489778	-2.072226	-0.015273	0.891926	
35.	1051.661284	0.871031	-0.018294	0.877068		35.	944.417552	-2.086968	-0.014742	0.916490	
36.	1052.532315	0.852985	-0.018046	0.933708		36.	942.330584	-2.106795	-0.019827	0.915463	
37.	1053.385300			0.924320		37.	940.223789			0.947051	

K=1 n=0 E2 (011)E2

R_branch

J	wv	delta1	delta2	intens	Comm
1.	1011.299052	1.495231		0.682722	
2.	1012.794283	1.477834	-0.017397	0.537550	c
3.	1014.272117	1.460279	-0.017555	0.422049	c
4.	1015.732396	1.442773	-0.017506	0.349106	
5.	1017.175169	1.424587	-0.018186	0.266474	c
6.	1018.599756	1.407003	-0.017584	0.217081	
7.	1020.006759	1.388426	-0.018577	0.192990	
8.	1021.395185	1.370562	-0.017864	0.200111	c
9.	1022.765747	1.352071	-0.018491	0.194524	c
10.	1024.117818	1.333582	-0.018489	0.192978	c
11.	1025.451400	1.314898	-0.018684	0.199936	c
12.	1026.766298	1.296275	-0.018623	0.172857	
13.	1028.062573	1.277255	-0.019020	0.202917	
14.	1029.339828	1.258439	-0.018816	0.206572	
15.	1030.598267	1.239902	-0.018537	0.087708	
16.	1031.838169	1.221654	-0.018248	0.229883	
17.	1033.059823	1.200755	-0.020899	0.160292	
18.	1034.260578	1.182725	-0.018030	0.298483	
19.	1035.443303	1.164228	-0.018497	0.335890	
20.	1036.607531	1.144826	-0.019402	0.225644	
21.	1037.752357	1.125954	-0.018872	0.201085	
22.	1038.878311	1.107270	-0.018684	0.457272	
23.	1039.985581	1.089006	-0.018264	0.454865	
24.	1041.074587	1.070213	-0.018793	0.545712	
25.	1042.144800	1.051871	-0.018342	0.552739	
26.	1043.196671	1.033499	-0.018372	0.627043	
27.	1044.230170	1.015235	-0.018264	0.683848	
28.	1045.245405	0.997034	-0.018201	0.722158	
29.	1046.242439	0.979020	-0.018014	0.759821	
30.	1047.221459	0.960913	-0.018107	0.793897	
31.	1048.182372	0.943133	-0.017780	0.808388	
32.	1049.125505	0.925181	-0.017952	0.848083	
33.	1050.050686	0.907386	-0.017795	0.890235	
34.	1050.958072	0.889777	-0.017609	0.902750	
35.	1051.847849	0.871794	-0.017983	0.921012	
36.	1052.719643	0.859973	-0.011821	0.931068	
37.	1053.579616			0.894648	

P_branch

J	wv	delta1	delta2	intens	Comm
2.	1005.147454	-1.580333		0.639769	
3.	1003.567121	-1.596593	-0.016260	0.526587	c
4.	1001.970528	-1.613008	-0.016415	0.431370	c
5.	1000.357520	-1.629337	-0.016329	0.356779	
6.	998.728183	-1.645488	-0.016151	0.293884	c
7.	997.082695	-1.661567	-0.016079	0.257998	
8.	995.421128	-1.677406	-0.015839	0.245676	
9.	993.743722	-1.693283	-0.015877	0.218382	c
10.	992.050439	-1.708957	-0.015674	0.210093	c
11.	990.341482	-1.724640	-0.015683	0.203705	c
12.	988.616842	-1.739924	-0.015284	0.196800	c
13.	986.876918	-1.754756	-0.014832	0.208740	
14.	985.122162	-1.771390	-0.016634	0.064177	
15.	983.350772	-1.785957	-0.014567	0.226459	
16.	981.564815	-1.801374	-0.015417	0.253773	
17.	979.763441	-1.815980	-0.014606	0.209072	
18.	977.947461	-1.831319	-0.015339	0.298999	
19.	976.116142	-1.846323	-0.015004	0.318841	
20.	974.269819	-1.860976	-0.014653	0.357360	
21.	972.408843	-1.876838	-0.015862	0.291396	
22.	970.532005	-1.891279	-0.014441	0.341522	
23.	968.640726	-1.906432	-0.015153	0.477271	
24.	966.734294	-1.921576	-0.015144	0.530754	
25.	964.812718	-1.936396	-0.014820	0.562242	
26.	962.876322	-1.951537	-0.015141	0.624557	
27.	960.924785	-1.966622	-0.015085	0.669698	
28.	958.958163	-1.981743	-0.015121	0.722002	
29.	956.976420	-1.996845	-0.015102	0.759568	
30.	954.979575	-2.011855	-0.015010	0.785689	
31.	952.967720	-2.027067	-0.015212	0.814240	
32.	950.940653	-2.042780	-0.015713	0.845866	
33.	948.897873	-2.056598	-0.013818	0.819351	
34.	946.841275	-2.072241	-0.015643	0.905469	
35.	944.769034	-2.087160	-0.014919	0.920812	
36.	942.681874	-2.102654	-0.015494	0.922019	
37.	940.579220	-2.116715	-0.014061	0.940906	
38.	938.462505			0.951227	

(011)E2

Q_branch

J	wv	delta1	delta2	intens	Comm
2.	1008.206159	-0.050797		0.797389	c
3.	1008.155362	-0.066925	-0.016128	0.845765	c
4.	1008.088437	-0.083347	-0.016422	0.561316	c
5.	1008.005090	-0.106664	-0.023317	0.268651	c
6.	1007.898426	-0.119290	-0.012626	0.288142	c
7.	1007.779136	-0.133271	-0.013981	0.334162	
8.	1007.645865	-0.152643	-0.019372	0.426155	c
9.	1007.493222	-0.169900	-0.017257	0.838723	c
10.	1007.323322	-0.188288	-0.018388	0.785636	c
11.	1007.135034	-0.199861	-0.011573	0.782358	c
12.	1006.935173			0.620641	c

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K=3      n=0    A+                                          (013)A+

 R_branch                                                   |  P_branch

 J         wv          delta1      delta2      intens   Comm   |    J         wv          delta1      delta2      intens   Comm
 3.    1014.194415   1.461660                0.476255    c     |
 4.    1015.656075   1.444293   -0.017367   0.270204    c     |    4.   1001.890737   -1.613936               0.498076    c
 5.    1017.100368   1.427395   -0.016898   0.192630    c     |    5.   1000.276801   -1.630585   -0.016649   0.298821    c
 6.    1018.527763   1.410106   -0.017289   0.154625    c     |    6.    998.646216   -1.647492   -0.016907   0.190280    c
 7.    1019.937869   1.392958   -0.017148   0.114251    c     |    7.    996.998724   -1.664235   -0.016743   0.130574    c
 8.    1021.330827   1.375677   -0.017281   0.087944    c     |    8.    995.334489   -1.681141   -0.016906   0.099402    c
 9.    1022.706504   1.358770   -0.016907   0.086031    c     |    9.    993.653348   -1.696956   -0.015815   0.060373    c
10.    1024.065274   1.340764   -0.018006   0.045021    c     |   10.    991.956392   -1.716451   -0.019495   0.046425    c
11.    1025.406038   1.324232   -0.016532   0.074498    c     |   11.    990.239941   -1.730293   -0.013842   0.027688    c
12.    1026.730270   1.305228   -0.019004   0.077008          |   12.    988.509648   -1.747902   -0.017609   0.045049    c
13.    1028.035498   1.286964   -0.018264   0.053128          |   13.    986.761746   -1.763997   -0.016095   0.038107
14.    1029.322462   1.271516   -0.015448   0.107788          |   14.    984.997749   -1.780560   -0.016563   0.056487
15.    1030.593978   1.253050   -0.018466   0.268978          |   15.    983.217189   -1.797288   -0.016728   0.058171
16.    1031.847028   1.235347   -0.017703   0.301236          |   16.    981.419901   -1.813758   -0.016470   0.082908
17.    1033.082375   1.216866   -0.018481   0.307157          |   17.    979.606143   -1.829229   -0.015471   0.133401
18.    1034.299241   1.199710   -0.017156   0.307673          |   18.    977.776914   -1.847314   -0.018085   0.137164
19.    1035.498951   1.181447   -0.018263   0.391048          |   19.    975.929600   -1.863104   -0.015790   0.278900
20.    1036.680398   1.163385   -0.018062   0.432785          |   20.    974.066496   -1.882913   -0.019809   0.358438
21.    1037.843783   1.145201   -0.018184   0.479064          |   21.    972.183583   -1.892964   -0.010051   0.272455
22.    1038.988984   1.127670   -0.017531   0.474427          |   22.    970.290619   -1.912046   -0.019082   0.462219
23.    1040.116654   1.109172   -0.018498   0.309723          |   23.    968.378573   -1.928056   -0.016010   0.501237
24.    1041.225826   1.093077   -0.016095   0.604402          |   24.    966.450517   -1.944370   -0.016314   0.489928
25.    1042.318903   1.077481   -0.015596   0.655495          |   25.    964.506147   -1.960189   -0.015819   0.466691
26.    1043.396384   1.062632   -0.014849   0.912201          |   26.    962.545958   -1.973633   -0.013444   0.359353
                                                               |   27.    960.572325   -1.976327   -0.002694   0.720893
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(013)A+

Q_branch

J	wv	delta1	delta2	intens	Comm
3.	1008.076436	-0.067673		0.139252	c
4.	1008.008763	-0.084400	-0.016727	0.218132	c
5.	1007.924363	-0.102157	-0.017757	0.031842	c
6.	1007.822206	-0.118931	-0.016774	0.151891	c
7.	1007.703275	-0.136141	-0.017210	0.269162	c
8.	1007.567134	-0.151567	-0.015426	0.421782	c
9.	1007.415567	-0.169151	-0.017584	0.549309	c
10.	1007.246416	-0.186214	-0.017063	0.594781	c
11.	1007.060202	-0.205951	-0.019737	0.506144	c
12.	1006.854251	-0.224019	-0.018068	0.755041	c
13.	1006.630232	-0.233214	-0.009195	0.523810	
14.	1006.397018			0.588573	

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K=3        n=0    A-                              (013)A-

  R_branch                                          |  P_branch

 J        wv          delta1       delta2       intens    Comm  |    J        wv          delta1        delta2       intens    Comm
 3.    1014.194415   1.461660                  0.476255    c    |
 4.    1015.656075   1.444293    -0.017367     0.270204    c    |    4.   1001.890737   -1.613936                   0.498076    c
 5.    1017.100368   1.427395    -0.016898     0.192630    c    |    5.   1000.276801   -1.630585    -0.016649     0.298821    c
 6.    1018.527763   1.410106    -0.017289     0.154625    c    |    6.    998.646216   -1.647492    -0.016907     0.190280    c
 7.    1019.937869   1.392958    -0.017148     0.114251    c    |    7.    996.998724   -1.664235    -0.016743     0.130574    c
 8.    1021.330827   1.375677    -0.017281     0.087944    c    |    8.    995.334489   -1.681141    -0.016906     0.099402    c
 9.    1022.706504   1.358770    -0.016907     0.086031    c    |    9.    993.653348   -1.696956    -0.015815     0.060373    c
10.    1024.065274   1.340764    -0.018006     0.045021    c    |   10.    991.956392   -1.716451    -0.019495     0.046425    c
11.    1025.406038   1.324232    -0.016532     0.074498         |   11.    990.239941   -1.730293    -0.013842     0.027688    c
12.    1026.730270   1.305228    -0.019004     0.077008         |   12.    988.509648   -1.747902    -0.017609     0.045049
13.    1028.035498   1.290403    -0.014825     0.053128         |   13.    986.761746   -1.763997    -0.016095     0.038107
14.    1029.325901   1.272366    -0.018037     0.258711         |   14.    984.997749   -1.783064    -0.019067     0.056487
15.    1030.598267   1.254157    -0.018209     0.087708         |   15.    983.214685   -1.798910    -0.015846     0.196588
16.    1031.852424   1.236658    -0.017499     0.233886         |   16.    981.415775   -1.818062    -0.019152     0.288885
17.    1033.089082   1.219268    -0.017390     0.312917         |   17.    979.597713   -1.830251    -0.012189     0.187081
18.    1034.308350   1.201909    -0.017359     0.363058         |   18.    977.767462   -1.847820    -0.017569     0.101886
19.    1035.510259   1.184347    -0.017562     0.399655         |   19.    975.919642   -1.866965    -0.019145     0.170142
20.    1036.694606   1.166895    -0.017452     0.416079         |   20.    974.052677   -1.884409    -0.017444     0.377005
21.    1037.861501   1.149302    -0.017593     0.459211         |   21.    972.168268   -1.899655    -0.015246     0.298038
22.    1039.010803   1.131866    -0.017436     0.479635         |   22.    970.268613   -1.917591    -0.017936     0.496481
23.    1040.142669   1.114194    -0.017672     0.507998         |   23.    968.351022   -1.934833    -0.017242     0.543604
24.    1041.256863   1.096618    -0.017576     0.563087         |   24.    966.416189   -1.951989    -0.017156     0.582655
25.    1042.353481   1.079055    -0.017563     0.647351         |   25.    964.464200   -1.969652    -0.017663     0.605547
26.    1043.432536   1.061541    -0.017514     0.687728         |   26.    962.494548   -1.987646    -0.017994     0.668391
27.    1044.494077   1.043948    -0.017593     0.728987         |   27.    960.506902   -2.003922    -0.016276     0.642683
28.    1045.538025   1.026138    -0.017810     0.755261         |   28.    958.502980   -2.022180    -0.018258     0.746247
29.    1046.564163   1.009058    -0.017080     0.694440         |   29.    956.480800   -2.039875    -0.017695     0.785613
30.    1047.573221   0.991155    -0.017903     0.817391         |   30.    954.440925   -2.057561    -0.017686     0.813259
31.    1048.564376   0.973467    -0.017688     0.863530         |   31.    952.383364   -2.075233    -0.017672     0.856307
32.    1049.537843   0.956063    -0.017404     0.856183         |   32.    950.308131   -2.093218    -0.017985     0.873696
33.    1050.493906   0.947453    -0.008610     0.899381         |   33.    948.214913   -2.110714    -0.017496     0.897224
34.    1051.441359   0.924245    -0.023208     0.953176         |   34.    946.104199   -2.127901    -0.017187     0.905445
35.    1052.365604                             0.911312         |   35.    943.976298   -2.144695    -0.016794     0.922198
                                                                |   36.    941.831603   -2.151534    -0.006839     0.899938
                                                                |   37.    939.680069                              0.950114
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(013)A-

Q_branch

J	wv	delta1	delta2	intens	Comm
3.	1008.076436	-0.067673		0.139252	c
4.	1008.008763	-0.084400	-0.016727	0.218132	c
5.	1007.924363	-0.102157	-0.017757	0.031842	c
6.	1007.822206	-0.118931	-0.016774	0.151891	c
7.	1007.703275	-0.136141	-0.017210	0.269162	c
8.	1007.567134	-0.151567	-0.015426	0.421782	c
9.	1007.415567	-0.169151	-0.017584	0.549309	c
10.	1007.246416	-0.186214	-0.017063	0.594781	c
11.	1007.060202	-0.201825	-0.015611	0.506144	
12.	1006.858377	-0.218686	-0.016861	0.785584	
13.	1006.639691	-0.242673	-0.023987	0.473170	
14.	1006.397018	-0.258534	-0.015861	0.588573	
15.	1006.138484	-0.273796	-0.015262	0.495564	
16.	1005.864688			0.586890	

```
K=5       n=0    E1                                              (015)E1

 R_branch                                                        |  P_branch

 J       wv         delta1       delta2        intens    Comm    |     J         wv          delta1        delta2        intens    Comm
 5.   1017.095752  1.427168                   0.548542           |
 6.   1018.522920  1.409584   -0.017584      0.411858           |     6.    998.646216   -1.647492                    0.190280
 7.   1019.932504  1.391952   -0.017632      0.272203     c     |     7.    996.998724   -1.664235   -0.016743       0.130574
 8.   1021.324456  1.374249   -0.017703      0.169803     c     |     8.    995.334489   -1.681141   -0.016906       0.099402     c
 9.   1022.698705  1.357702   -0.016547      0.072253     c     |     9.    993.653348   -1.696956   -0.015815       0.060373     c
10.   1024.056407  1.336889   -0.020813      0.288415     c     |    10.    991.956392   -1.716451   -0.019495       0.046425     c
11.   1025.393296  1.317899   -0.018990      0.383790     c     |    11.    990.239941   -1.730293   -0.013842       0.027688     c
12.   1026.711195  1.305540   -0.012359      0.148537           |    12.    988.509648   -1.747902   -0.017609       0.045049     c
13.   1028.016735  1.287011   -0.018529      0.108650           |    13.    986.761746   -1.763997   -0.016095       0.038107
14.   1029.303746  1.267851   -0.019160      0.090431           |    14.    984.997749   -1.780560   -0.016563       0.056487
15.   1030.571597  1.249525   -0.018326      0.349046           |    15.    983.217189   -1.797288   -0.016728       0.058171
16.   1031.821122  1.232119   -0.017406      0.418527           |    16.    981.419901   -1.813758   -0.016470       0.082908
17.   1033.053241  1.214199   -0.017920      0.436915     c     |    17.    979.606143   -1.829229   -0.015471       0.133401
18.   1034.267440  1.196341   -0.017858      0.471578           |    18.    977.776914   -1.851688   -0.022459       0.137164     c
19.   1035.463781  1.178078   -0.018263      0.477890           |    19.    975.925226   -1.862208   -0.010520       0.290735
20.   1036.641859  1.160079   -0.017999      0.544900     c     |    20.    974.063018   -1.879435   -0.017227       0.507399
21.   1037.801938  1.142050   -0.018029      0.555569     c     |    21.    972.183583   -1.897144   -0.017709       0.272455     c
22.   1038.943988  1.123818   -0.018232      0.622796           |    22.    970.286439   -1.912654   -0.015510       0.588731     c
23.   1040.067806  1.105741   -0.018077      0.647640           |    23.    968.373785   -1.929055   -0.016401       0.629434
24.   1041.173547  1.087369   -0.018372      0.592981           |    24.    966.444730   -1.945122   -0.016067       0.628686
25.   1042.260916  1.067732   -0.019637      0.712490           |    25.    964.499608   -1.961281   -0.016159       0.694031
26.   1043.328648  1.052277   -0.015455      0.487074           |    26.    962.538327   -1.977571   -0.016290       0.748090
27.   1044.380925  1.032235   -0.020042      0.772432           |    27.    960.560756   -1.993631   -0.016060       0.772829
28.   1045.413160  1.014003   -0.018232      0.810337           |    28.    958.567125   -2.009727   -0.016096       0.811349
29.   1046.427163  0.996036   -0.017967      0.809793           |    29.    956.557398   -2.026930   -0.017203       0.837117
30.   1047.423199  0.976681   -0.019355      0.726668           |    30.    954.530468   -2.039540   -0.012610       0.782268
31.   1048.399880  0.958558   -0.018123      0.864640           |    31.    952.490928   -2.058485   -0.018945       0.767044
32.   1049.358438  0.939046   -0.019512      0.830710           |    32.    950.432443   -2.075139   -0.016654       0.819363
33.   1050.297484  0.923201   -0.015845      0.860652           |    33.    948.357304   -2.088738   -0.013599       0.869269
34.   1051.220685                             0.921778           |    34.    946.268566   -2.097091   -0.008353       0.937812
                                                                 |    35.    944.171475                                0.906978
```

(015)E1

Q_branch

J	wv	delta1	delta2	intens	Comm
5.	1007.920284	-0.101759		0.360293	
6.	1007.818525	-0.118634	-0.016875	0.442653	
7.	1007.699891	-0.132757	-0.014123	0.177669	c
8.	1007.567134	-0.155162	-0.022405	0.421782	c
9.	1007.411972	-0.170469	-0.015307	0.249350	c
10.	1007.241503	-0.187196	-0.016727	0.381152	c
11.	1007.054307	-0.205936	-0.018740	0.420108	c
12.	1006.848371	-0.225859	-0.019923	0.344197	
13.	1006.622512	-0.234516	-0.008657	0.313428	
14.	1006.387996	-0.278529	-0.028439	0.726666	
15.	1006.093893	-0.307842	-0.029313	0.556408	
16.	1005.786051	-0.218382	0.089460	0.831346	
17.	1005.567669	-0.307070	-0.088688	0.395971	c
18.	1005.260599	-0.366469	-0.017171	0.623628	
19.	1004.738040	-0.146264	0.220205	0.879674	
20.	1004.591776	-0.359295	-0.213031	0.864167	c
21.	1004.232481	-0.374931	-0.015636	0.891594	c
22.	1003.857550			0.894660	

K=6 n=0 A (016)A

R_branch						P_branch					
J	wv	delta1	delta2	intens	Comm	J	wv	delta1	delta2	intens	Comm
6.	1018.539320	1.408874		0.653889							
7.	1019.948194	1.391710	-0.017164	0.470998	c	7.	997.017424	-1.664562		0.194420	
8.	1021.339904	1.373867	-0.017843	0.295457	c	8.	995.352862	-1.680806	-0.016244	0.496643	c
9.	1022.713771	1.356782	-0.017085	0.328211	c	9.	993.672056	-1.697486	-0.016680	0.391413	c
10.	1024.070553	1.338581	-0.018201	0.185864	c	10.	991.974570	-1.714042	-0.016556	0.335526	c
11.	1025.409134	1.321136	-0.017445	0.093817	c	11.	990.260528	-1.730636	-0.016594	0.298807	c
12.	1026.730270	1.305228	-0.015908	0.077008	c	12.	988.529892	-1.747137	-0.016501	0.275314	c
13.	1028.035498	1.286964	-0.018264	0.053128	c	13.	986.782755	-1.764036	-0.016899	0.246377	c
14.	1029.322462	1.268334	-0.018630	0.107788	c	14.	985.018719	-1.779766	-0.015730	0.093830	c
15.	1030.590796	1.251241	-0.017093	0.236795	c	15.	983.238953	-1.796578	-0.016812	0.274211	c
16.	1031.842037	1.233351	-0.017890	0.264357	c	16.	981.442375	-1.812892	-0.016314	0.275202	c
17.	1033.075388	1.215650	-0.017701	0.283708	c	17.	979.629483	-1.829252	-0.016360	0.303015	c
18.	1034.291038	1.197838	-0.017812	0.319495	c	18.	977.800231	-1.845520	-0.016268	0.324391	c
19.	1035.488876	1.180011	-0.017827	0.347943	c	19.	975.954711	-1.861787	-0.016267	0.344090	c
20.	1036.668887	1.162217	-0.017794	0.330249	c	20.	974.092924	-1.877992	-0.016205	0.379443	c
21.	1037.831104	1.143718	-0.018499	0.309124	c	21.	972.214932	-1.894149	-0.016157	0.417088	c
22.	1038.974822	1.126516	-0.017202	0.412844	c	22.	970.320783	-1.910292	-0.016143	0.446782	c
23.	1040.101338	1.108237	-0.018279	0.511552	c	23.	968.410491	-1.926278	-0.015986	0.490903	c
24.	1041.209575	1.086713	-0.021524	0.547282	c	24.	966.484213	-1.942713	-0.016435	0.507399	c
25.	1042.296288	1.074939	-0.011774	0.398465	c	25.	964.541500	-1.957966	-0.015253	0.345497	c
26.	1043.371227	1.055021	-0.019918	0.421122	c	26.	962.583534	-1.974589	-0.016623	0.529398	c
27.	1044.426248	1.035838	-0.019183	0.454950	c	27.	960.608945	-1.989853	-0.015264	0.657012	c
28.	1045.462086	1.017372	-0.018466	0.535062		28.	958.619092	-2.005719	-0.015866	0.714276	c
29.	1046.479458	1.000575	-0.016797	0.673238		29.	956.613373	-2.021681	-0.015962	0.620980	
30.	1047.480033	0.981921	-0.018654	0.796179		30.	954.591692	-2.037360	-0.015679	0.784384	
31.	1048.461954	0.964172	-0.017749	0.829844		31.	952.554332	-2.052516	-0.015156	0.825068	
32.	1049.426126	0.946143	-0.018029	0.853963		32.	950.501816	-2.068292	-0.015776	0.834490	
33.	1050.372269	0.928659	-0.017484	0.881323		33.	948.433524	-2.083455	-0.015163	0.878327	
34.	1051.300928	0.910911	-0.017748	0.909389		34.	946.350069	-2.098209	-0.014754	0.837247	
35.	1052.211839			0.909388		35.	944.251860	-2.112921	-0.014712	0.917590	

(016)A

Q_branch

J	wv	delta1	delta2	intens	Comm
6.	1007.841943	-0.123415		0.381817	
7.	1007.718528	-0.136110	-0.012695	0.125538	c
8.	1007.582418	-0.153094	-0.016984	0.167303	c
9.	1007.429324	-0.170220	-0.017126	0.232872	c
10.	1007.259104	-0.186939	-0.016719	0.314396	c
11.	1007.072165	-0.204813	-0.017874	0.331560	c
12.	1006.867352	-0.220884	-0.016071	0.221168	c
13.	1006.646468	-0.238330	-0.017446	0.490331	c
14.	1006.408138	-0.255298	-0.016968	0.538841	c
15.	1006.152840	-0.272337	-0.017039	0.447877	c
16.	1005.880503	-0.289587	-0.017250	0.606202	c
17.	1005.590916	-0.306221	-0.016634	0.673128	c
18.	1005.284695	-0.324063	-0.017842	0.572768	c
19.	1004.960632	-0.340197	-0.016134	0.733286	c
20.	1004.620435	-0.357128	-0.016931	0.789520	c
21.	1004.263307	-0.374821	-0.017693	0.830107	c
22.	1003.888486	-0.389756	-0.014935	0.866638	c
23.	1003.498730	-0.410709	-0.020953	0.588360	c
24.	1003.088021	-0.426796	-0.016087	0.875964	c
25.	1002.661225	-0.440748	-0.013952	0.880405	c
26.	1002.220477	-0.461608	-0.020860	0.943587	c
27.	1001.758869	-0.474249	-0.012641	0.625149	c
28.	1001.284620			0.896860	c

K=3   n=0   E2   (023)E2

R_branch						P_branch					
J	wv	delta1	delta2	intens	Comm	J	wv	delta1	delta2	intens	Comm
3.	1014.063795	1.462042		0.703548							
4.	1015.525837	1.445112	-0.016930	0.549469		4.	1001.758869	-1.613570		0.625149	
5.	1016.970949	1.428034	-0.017078	0.447692		5.	1000.145299	-1.630187	-0.016617	0.544680	
6.	1018.398983	1.410948	-0.017086	0.384300		6.	998.515112	-1.646813	-0.016626	0.458841	
7.	1019.809931	1.393699	-0.017249	0.095409		7.	996.868299	-1.663408	-0.016595	0.398014	
8.	1021.203630	1.376558	-0.017141	0.313295	c	8.	995.204891	-1.679597	-0.016189	0.345711	
9.	1022.580188	1.359246	-0.017312	0.294261	c	9.	993.525294	-1.696925	-0.017328	0.211162	c
10.	1023.939434	1.341988	-0.017258	0.278582	c	10.	991.828369	-1.713028	-0.016103	0.295617	c
11.	1025.281422	1.324591	-0.017397	0.277325	c	11.	990.115341	-1.729529	-0.016501	0.286274	c
12.	1026.606013	1.307208	-0.017383	0.240680	c	12.	988.385812	-1.745999	-0.016470	0.285428	c
13.	1027.913221	1.289959	-0.017249	0.282682	c	13.	986.639813	-1.762406	-0.016407	0.279635	c
14.	1029.203180	1.272000	-0.017959	0.179601	c	14.	984.877407	-1.778985	-0.016579	0.288940	c
15.	1030.475180	1.254359	-0.017641	0.306190	c	15.	983.098422	-1.795268	-0.016283	0.090683	c
16.	1031.729539	1.237189	-0.017170	0.107564		16.	981.303154	-1.811660	-0.016392	0.298264	c
17.	1032.966728	1.221357	-0.015832	0.103519		17.	979.491494	-1.828076	-0.016416	0.318321	
18.	1034.188085	1.199632	-0.021725	0.287611		18.	977.663418	-1.844396	-0.016320	0.358370	
19.	1035.387717	1.183786	-0.015846	0.403163		19.	975.819022	-1.860742	-0.016346	0.403479	
20.	1036.571503	1.165913	-0.017873	0.440108		20.	973.958280	-1.877103	-0.016361	0.436517	
21.	1037.737416	1.148132	-0.017781	0.488663		21.	972.081177	-1.893440	-0.016337	0.457209	
22.	1038.885548	1.129947	-0.018185	0.517341		22.	970.187737	-1.909785	-0.016345	0.509444	
23.	1040.015495	1.111996	-0.017951	0.546689		23.	968.277952	-1.926099	-0.016314	0.544925	
24.	1041.127491	1.093950	-0.018046	0.617380		24.	966.351853	-1.942369	-0.016270	0.602421	
25.	1042.221441	1.075936	-0.018014	0.619836		25.	964.409484	-1.958727	-0.016358	0.634518	
26.	1043.297377	1.057627	-0.018309	0.652444		26.	962.450757	-1.975040	-0.016313	0.676681	
27.	1044.355004	1.038988	-0.018639	0.723110		27.	960.475717	-1.991359	-0.016319	0.719350	
28.	1045.393992	1.021708	-0.017280	0.600252		28.	958.484358	-2.007773	-0.016414	0.747885	
29.	1046.415700	1.002976	-0.018732	0.805025		29.	956.476585	-2.023982	-0.016209	0.787944	
30.	1047.418676	0.984776	-0.018200	0.777478		30.	954.452603	-2.040600	-0.016618	0.822818	
31.	1048.403452	0.966106	-0.018670	0.862907		31.	952.412003	-2.057004	-0.016404	0.853332	
32.	1049.369558	0.947687	-0.018419	0.886564		32.	950.354999	-2.073563	-0.016559	0.878609	
33.	1050.317245	0.930000	-0.017687	0.883800		33.	948.281436	-2.090213	-0.016650	0.903961	
34.	1051.247245	0.911566	-0.018434	0.905029		34.	946.191223	-2.106787	-0.016574	0.898987	
35.	1052.158811	0.892818	-0.018748	0.935280		35.	944.084436	-2.123929	-0.017142	0.937505	
36.	1053.051629	0.875445	-0.017373	0.866443		36.	941.960507	-2.148020	-0.024091	0.944509	
37.	1053.927074			0.921684		37.	939.812487			0.945380	

```
            (023)E2

| Q_branch
|   J        wv         delta1      delta2      intens   Comm
|
|
|
|
|
|   8.   1007.439937  -0.151527              0.188149    c
|   9.   1007.288410  -0.168356  -0.016829   0.191218    c
|  10.   1007.120054  -0.184881  -0.016525   0.779114    c
|  11.   1006.935173  -0.202730  -0.017849   0.620641    c
|  12.   1006.732443  -0.220074  -0.017344   0.835427    c
|  13.   1006.512369  -0.235163  -0.015089   0.530766    c
|  14.   1006.277206  -0.253645  -0.018482   0.878013    c
|  15.   1006.023561  -0.269397  -0.015752   0.800137    c
|  16.   1005.754164                         0.505736    c
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K=4       n=0    E1                                          (024)E1

 R_branch                                                   |  P_branch

 J        wv         delta1      delta2       intens   Comm  |   J        wv          delta1      delta2      intens    Comm
 4.    1015.573578  1.444535                 0.724490        |
 5.    1017.018113  1.427566  -0.016969    0.595500     c   |    5.   1000.194709  -1.630461                0.711106
 6.    1018.445679  1.410012  -0.017554    0.466641     c   |    6.    998.564248  -1.646984  -0.016523   0.579502    c
 7.    1019.855691  1.393535  -0.016477    0.401719     c   |    7.    996.917264  -1.663689  -0.016705   0.504120    c
 8.    1021.249226  1.376004  -0.017531    0.299412     c   |    8.    995.253575  -1.680275  -0.016586   0.401197    c
 9.    1022.625230  1.358654  -0.017350    0.355367     c   |    9.    993.573300  -1.696995  -0.016720   0.384340    c
10.    1023.983884  1.341201  -0.017453    0.337332     c   |   10.    991.876305  -1.714050  -0.017055   0.351988    c
11.    1025.325085  1.324044  -0.017157    0.197646     c   |   11.    990.162255  -1.729513  -0.015463   0.246086    c
12.    1026.649129  1.306507  -0.017537    0.321907     c   |   12.    988.432742  -1.746623  -0.017110   0.342746    c
13.    1027.955636  1.288914  -0.017593    0.336099     c   |   13.    986.686119  -1.763147  -0.016524   0.313635    c
14.    1029.244550  1.271461  -0.017453    0.325130         |   14.    984.922972  -1.780327  -0.017180   0.343433    c
15.    1030.516011  1.253892  -0.017569    0.349936         |   15.    983.142645  -1.795463  -0.015136   0.134194
16.    1031.769903  1.236393  -0.017499    0.378456         |   16.    981.347182  -1.812658  -0.017195   0.377303
17.    1033.006296  1.218254  -0.018139    0.321225         |   17.    979.534524  -1.829026  -0.016368   0.362068
18.    1034.224550  1.200724  -0.017530    0.430481         |   18.    977.705498  -1.845481  -0.016455   0.422669
19.    1035.425274  1.182257  -0.018467    0.458827         |   19.    975.860017  -1.861974  -0.016493   0.453230
20.    1036.607531  1.165616  -0.016641    0.225644         |   20.    973.998043  -1.878553  -0.016579   0.481438
21.    1037.773147  1.147010  -0.018606    0.532615         |   21.    972.119490  -1.894462  -0.015909   0.243546
22.    1038.920157  1.129073  -0.017937    0.580225         |   22.    970.225028  -1.911141  -0.016679   0.546244
23.    1040.049230  1.110966  -0.018107    0.603277         |   23.    968.313887  -1.927534  -0.016393   0.594698
24.    1041.160196  1.092687  -0.018279    0.639339         |   24.    966.386353  -1.943797  -0.016263   0.632506
25.    1042.252883  1.075765  -0.016922    0.689205         |   25.    964.442556  -1.960349  -0.016552   0.668781
26.    1043.328648  1.055069  -0.020696    0.487074         |   26.    962.482207  -1.975305  -0.014956   0.711567
27.    1044.383717  1.035354  -0.019715    0.702806         |   27.    960.506902  -1.994178  -0.018873   0.642683
28.    1045.419071  1.015126  -0.020228    0.872199         |   28.    958.512724  -2.009391  -0.015213   0.773234
29.    1046.434197  0.989002  -0.026124    0.776190         |   29.    956.503333  -2.025718  -0.016327   0.813078
30.    1047.423199  0.971565  -0.017437    0.726668         |   30.    954.477615  -2.041992  -0.016274   0.852532
31.    1048.394764                          0.824693         |   31.    952.435623  -2.058411  -0.016419   0.871575
                                                             |   32.    950.377212  -2.074858  -0.016447   0.895221
                                                             |   33.    948.302354  -2.091401  -0.016543   0.917014
                                                             |   34.    946.210953  -2.107825  -0.016424   0.927206
                                                             |   35.    944.103128  -2.124221  -0.016396   0.934360
                                                             |   36.    941.978907  -2.141770  -0.017549   0.952287
                                                             |   37.    939.837137  -2.161718  -0.019948   0.952601
                                                             |   38.    937.675419  -2.189718  -0.028000   0.952074
                                                             |   39.    935.485701                          0.947745
```

(024)E1

Q_branch

J	wv	delta1	delta2	intens	Comm
5.	1007.841943	-0.101743		0.381817	c
6.	1007.740200	-0.117863	-0.016120	0.391349	c
7.	1007.622337	-0.134776	-0.016913	0.535628	c
8.	1007.487561	-0.152346	-0.017570	0.346708	c
9.	1007.335215	-0.168208	-0.015862	0.638858	c
10.	1007.167007	-0.186612	-0.018404	0.524097	c
11.	1006.980395	-0.202886	-0.016274	0.722484	c
12.	1006.777509	-0.220035	-0.017149	0.537771	c
13.	1006.557474	-0.235935	-0.015900	0.786129	c
14.	1006.321539			0.467137	c

```
K=6        n=0    E2                                          (026)E2

  R_branch                                                  |  P_branch

 J       wv          delta1      delta2       intens   Comm |   J        wv         delta1      delta2       intens    Comm
 6.    1018.599756   1.407003                 0.217081      |
 7.    1020.006759   1.392583   -0.014420     0.192990      |   7.    997.078227  -1.664461                 0.802967
 8.    1021.399342   1.374351   -0.018232     0.594217      |   8.    995.413766  -1.683059   -0.018598     0.698170
 9.    1022.773693   1.356446   -0.017905     0.478409      |   9.    993.730707  -1.696044   -0.012985     0.577126
10.    1024.130139   1.338909   -0.017537     0.119537      |  10.    992.034663  -1.716389   -0.020345     0.556534
11.    1025.469048   1.321728   -0.017181     0.491292   c  |  11.    990.318274  -1.729739   -0.013350     0.184064
12.    1026.790776   1.304238   -0.017490     0.489925   c  |  12.    988.588535  -1.748042   -0.018303     0.509322    c
13.    1028.095014   1.286769   -0.017469     0.437431   c  |  13.    986.840493  -1.764247   -0.016205     0.507230    c
14.    1029.381783   1.269184   -0.017585     0.493769   c  |  14.    985.076246  -1.781590   -0.017343     0.425812    c
15.    1030.650967   1.251880   -0.017304     0.488678   c  |  15.    983.294656  -1.797771   -0.016181     0.508704    c
16.    1031.902847   1.235052   -0.016828     0.162410   c  |  16.    981.496885  -1.814202   -0.016431     0.520425    c
17.    1033.137899   1.215119   -0.019933     0.262668      |  17.    979.682683  -1.830836   -0.016634     0.503012    c
18.    1034.353018   1.198696   -0.016423     0.534593      |  18.    977.851847  -1.847173   -0.016337     0.545487
19.    1035.551714   1.181025   -0.017671     0.584302      |  19.    976.004674  -1.863620   -0.016447     0.571075
20.    1036.732739   1.163277   -0.017748     0.516101      |  20.    974.141054  -1.879878   -0.016258     0.582207
21.    1037.896016   1.145512   -0.017765     0.642569      |  21.    972.261176  -1.896263   -0.016385     0.638537
22.    1039.041528   1.127626   -0.017686     0.679869      |  22.    970.364913  -1.912585   -0.016322     0.645786
23.    1040.169354   1.109968   -0.017858     0.705442      |  23.    968.452328  -1.928695   -0.016110     0.694512
24.    1041.279322   1.092188   -0.017780     0.736174      |  24.    966.523633  -1.945033   -0.016338     0.723299
25.    1042.371510   1.074439   -0.017749     0.765498      |  25.    964.578600  -1.959526   -0.014493     0.745968
26.    1043.445949   1.056332   -0.018107     0.800941      |  26.    962.619074  -1.979100   -0.019574     0.666951
27.    1044.502281   1.039503   -0.016829     0.805693      |  27.    960.639974  -1.993771   -0.014671     0.618970
28.    1045.541784   1.022379   -0.017124     0.841288      |  28.    958.646203  -2.007918   -0.014147     0.678001
29.    1046.564163   1.000122   -0.022257     0.694440      |  29.    956.638285  -2.024844   -0.016926     0.865128
30.    1047.564285   0.974325   -0.025797     0.779806      |  30.    954.613441  -2.040132   -0.015288     0.881355
31.    1048.538610   0.986647    0.012322     0.860661      |  31.    952.573309  -2.055522   -0.015390     0.904022
32.    1049.525257   1.006642    0.019995     0.762704      |  32.    950.517787  -2.070460   -0.014938     0.911682
33.    1050.531899                            0.957715      |  33.    948.447327  -2.087019   -0.016559     0.934790
                                                            |  34.    946.360308                            0.904940
```

(026)E2

Q_branch

J	wv	delta1	delta2	intens	Comm
11.	1007.131151	-0.204641		0.546925	c
12.	1006.926510	-0.221680	-0.017039	0.647296	c
13.	1006.704830	-0.237402	-0.015722	0.692078	c
14.	1006.467428	-0.257435	-0.020033	0.490628	c
15.	1006.209993	-0.272774	-0.015339	0.739081	c
16.	1005.937219	-0.289524	-0.016750	0.551493	c
17.	1005.647695			0.796979	c

K=0   n=0   E1   (030)E

R_branch

J	wv	delta1	delta2	intens	Comm
0.	1009.592387	1.512809		0.785645	
1.	1011.105196	1.495519	-0.017290	0.622406	
2.	1012.600715	1.478045	-0.017474	0.497608	
3.	1014.078760	1.460045	-0.018000	0.386458	
4.	1015.538805	1.442071	-0.017974	0.340290	
5.	1016.980876	1.423823	-0.018248	0.292493	
6.	1018.404699	1.405232	-0.018591	0.253688	
7.	1019.809931	1.386657	-0.018575	0.095409	
8.	1021.196588	1.368456	-0.018201	0.199045	
9.	1022.565044	1.348414	-0.020042	0.049603	
10.	1023.913458	1.329215	-0.019199	0.068616	
11.	1025.242673	1.310390	-0.018825	0.192968	
12.	1026.553063	1.291596	-0.018794	0.189987	
13.	1027.844659	1.272460	-0.019136	0.198815	
14.	1029.117119	1.253502	-0.018958	0.213417	
15.	1030.370621	1.234833	-0.018669	0.229781	
16.	1031.605454	1.216227	-0.018606	0.177936	
17.	1032.821681	1.197713	-0.018514	0.251584	
18.	1034.019394	1.179653	-0.018060	0.279397	
19.	1035.199047	1.161602	-0.018051	0.344182	
20.	1036.360649	1.143506	-0.018096	0.329184	
21.	1037.504155	1.125471	-0.018035	0.386797	
22.	1038.629626	1.108003	-0.017468	0.347028	
23.	1039.737629	1.090098	-0.017905	0.506552	
24.	1040.827727	1.072412	-0.017686	0.538891	
25.	1041.900139	1.054585	-0.017827	0.592379	
26.	1042.954724	1.036914	-0.017671	0.648557	
27.	1043.991638	1.019087	-0.017827	0.670871	
28.	1045.010725	1.001276	-0.017811	0.705152	
29.	1046.012001	0.983731	-0.017545	0.769861	
30.	1046.995732	0.965373	-0.018358	0.745852	
31.	1047.961105	0.947687	-0.017686	0.824835	
32.	1048.908792	0.929720	-0.017967	0.851389	
33.	1049.838512	0.911768	-0.017952	0.876986	
34.	1050.750280	0.893505	-0.018263	0.900839	
35.	1051.643785	0.876115	-0.017390	0.920495	
36.	1052.519900	0.857321	-0.018794	0.934638	
37.	1053.377221	0.830183	-0.027138	0.954441	
38.	1054.207404			0.885321	

P_branch

J	wv	delta1	delta2	intens	Comm
1.	1006.519466	-1.566921		0.572559	
2.	1004.952545	-1.579483	-0.012562	0.615754	
3.	1003.373062	-1.595431	-0.015948	0.483405	
4.	1001.777631	-1.611347	-0.015916	0.371291	
5.	1000.166284	-1.626701	-0.015354	0.345987	
6.	998.539583	-1.641971	-0.015270	0.296869	
7.	996.897612	-1.656943	-0.014972	0.269176	
8.	995.240669	-1.671721	-0.014778	0.240250	
9.	993.568948	-1.686272	-0.014551	0.217431	
10.	991.882676	-1.700707	-0.014435	0.216594	
11.	990.181969	-1.715009	-0.014302	0.206130	
12.	988.466960	-1.729419	-0.014410	0.208460	
13.	986.737541	-1.743161	-0.013742	0.211746	
14.	984.994380	-1.759341	-0.016180	0.172700	
15.	983.235039	-1.771998	-0.012657	0.075869	
16.	981.463041	-1.788024	-0.016026	0.093768	
17.	979.675017	-1.802216	-0.014192	0.175447	
18.	977.872801	-1.817907	-0.015691	0.305192	
19.	976.054894	-1.833385	-0.015478	0.334598	
20.	974.221509	-1.849224	-0.015839	0.373774	
21.	972.372285	-1.864594	-0.015370	0.213399	
22.	970.507691	-1.881283	-0.016689	0.302957	
23.	968.626408	-1.897082	-0.015799	0.492490	
24.	966.729326	-1.913309	-0.016227	0.542743	
25.	964.816017	-1.929581	-0.016272	0.582346	
26.	962.886436	-1.945770	-0.016189	0.637577	
27.	960.940666	-1.961386	-0.015616	0.683845	
28.	958.979280	-1.978584	-0.017198	0.565629	
29.	957.000696	-1.994361	-0.015777	0.750821	
30.	955.006335	-2.010265	-0.015904	0.793853	
31.	952.996070	-2.026415	-0.016150	0.825276	
32.	950.969655	-2.042238	-0.015823	0.858548	
33.	948.927417	-2.058092	-0.015854	0.865596	
34.	946.869325	-2.073925	-0.015833	0.904433	
35.	944.795400	-2.089499	-0.015574	0.916801	
36.	942.705901			0.930423	

K=5 n=0 E2 (035)E2

R_branch

J	wv	delta1	delta2	intens	Comm
5.	1016.935647	1.427823		0.752472	c
6.	1018.363470	1.407774	-0.020049	0.223020	c
7.	1019.771244	1.391835	-0.015939	0.538795	c
8.	1021.163079	1.374718	-0.017117	0.463053	c
9.	1022.537797	1.357109	-0.017609	0.391154	
10.	1023.894906	1.339657	-0.017452	0.384100	
11.	1025.234563	1.322407	-0.017250	0.388059	c
12.	1026.556970	1.304775	-0.017632	0.385661	c
13.	1027.861745	1.287316	-0.017459	0.383996	
14.	1029.149061	1.269753	-0.017563	0.391489	c
15.	1030.418814	1.252379	-0.017374	0.412323	c
16.	1031.671193	1.234256	-0.018123	0.292232	c
17.	1032.905449	1.216726	-0.017530	0.437019	c
18.	1034.122175	1.199070	-0.017656	0.461675	
19.	1035.321245	1.181244	-0.017826	0.463786	
20.	1036.502489	1.163292	-0.017952	0.495581	
21.	1037.665781	1.145341	-0.017951	0.566984	
22.	1038.811122	1.128060	-0.017281	0.591718	
23.	1039.939182	1.109391	-0.018669	0.358014	
24.	1041.048573	1.091782	-0.017609	0.673768	
25.	1042.140355	1.072958	-0.018824	0.707450	
26.	1043.213313	1.055536	-0.017422	0.740337	
27.	1044.268849	1.037226	-0.018310	0.758308	
28.	1045.306075	1.019244	-0.017982	0.804152	
29.	1046.325319	1.000979	-0.018265	0.815091	
30.	1047.326298	0.982764	-0.018215	0.856984	
31.	1048.309062			0.876332	

P_branch

J	wv	delta1	delta2	intens	Comm
6.	998.486477	-1.648139		0.758371	c
7.	996.838338	-1.663821	-0.015682	0.189422	c
8.	995.174517	-1.681219	-0.017398	0.541212	c
9.	993.493298	-1.697869	-0.016650	0.476969	c
10.	991.795429	-1.714657	-0.016788	0.426428	
11.	990.080772	-1.731541	-0.016884	0.389787	
12.	988.349231	-1.748136	-0.016595	0.397904	c
13.	986.601095	-1.764769	-0.016633	0.380530	c
14.	984.836326	-1.780444	-0.015675	0.333168	
15.	983.055882	-1.799284	-0.018840	0.193820	c
16.	981.256598	-1.816869	-0.017585	0.134669	c
17.	979.439729	-1.829323	-0.012454	0.081400	c
18.	977.610406	-1.848023	-0.018700	0.451722	c
19.	975.762383	-1.864610	-0.016587	0.502319	
20.	973.897773	-1.881189	-0.016579	0.526464	
21.	972.016584	-1.897713	-0.016524	0.564379	
22.	970.118871	-1.914331	-0.016618	0.595595	
23.	968.204540	-1.930755	-0.016424	0.637357	
24.	966.273785	-1.947333	-0.016578	0.669913	
25.	964.326452	-1.963811	-0.016478	0.693673	
26.	962.362641	-1.979934	-0.016123	0.734873	
27.	960.382707	-1.997160	-0.017226	0.780559	
28.	958.385547	-2.013205	-0.016045	0.771466	
29.	956.372342	-2.029581	-0.016376	0.830546	
30.	954.342761	-2.045899	-0.016318	0.865747	
31.	952.296862	-2.061792	-0.015893	0.886320	
32.	950.235070	-2.078741	-0.016949	0.786002	
33.	948.156329	-2.094354	-0.015613	0.919047	
34.	946.061975			0.931037	

(035)E2

Q_branch

J	wv	delta1	delta2	intens	Comm
5.	1007.762105	-0.102149		0.266920	c
6.	1007.659956	-0.119055	-0.016906	0.337206	c
7.	1007.540901	-0.136563	-0.017508	0.389555	c
8.	1007.404338	-0.153297	-0.016734	0.154966	c
9.	1007.251041	-0.172918	-0.019621	0.204014	
10.	1007.078123	-0.184927	-0.012009	0.404781	
11.	1006.893196	-0.203214	-0.018287	0.499294	c
12.	1006.689982	-0.222554	-0.019340	0.564751	c
13.	1006.467428	-0.238984	-0.016430	0.490628	
14.	1006.228444	-0.253637	-0.014653	0.458375	c
15.	1005.974807	-0.273461	-0.019824	0.462291	c
16.	1005.701346	-0.291240	-0.017779	0.772308	c
17.	1005.410106	-0.305597	-0.014357	0.810964	c
18.	1005.104509			0.696886	

B.4 Sample section of the new.ass_pkf output

The following sample section is only the record of line 1019.771244 to line 1020.006759 from the output file new.ass_pkf of the spectrum of CD_3OH in the 910-1300 cm^{-1} region. Section 6.1.1 gives a detailed description of this file.

```
1019.771244     0.538795 1 OH 0 0 5 E2 R 7 c
1019.787987     0.268836
1019.792861     0.249195
1019.795973     0.250349
1019.809931     0.095409 1 OH 0 0 3 E2 R 7  1 OH 0 0 0 E1 R 7 o
1019.814797     0.958477
1019.821839     0.815749
1019.830285     0.633906
1019.849632     0.550851
1019.855691     0.401719 1 OH 0 0 4 E1 R 7 c
1019.872925     0.947464
1019.880006     0.748280
1019.884911     0.920173
1019.923668     0.118464
1019.932504     0.272203
1019.937869     0.114251
1019.948194     0.470998
1019.960351     0.198658
1019.967822     0.164375
1019.974100     0.310232
1019.987520     0.703466
1020.006759     0.192990 1 OH 0 0 1 E2 R 7
```

B.5 Samples of unsuccessful series assignments in the spectrum of $CH_3^{18}OH$ in the 900-1100 cm^{-1} region.

This appendix gives the unsuccessful series assignments by MOSAA. Only the R branches are found for these series while the corresponding P branch couldn't be found. Failure of assigning (014)E2 was due to the high bias in calculated R-P Combination differences. Failure of assigning the other series was due to the failure of RPQ confirmation.

(012)E1

R branch

J	wv	delta1	delta2	intens
6	1018.546401	1.413950		0.130159
7.	1019.960351	1.395882	-0.018068	0.198658
8.	1021.356233	1.379451	-0.016431	0.245442
9.	1022.735684	1.362085	-0.017366	0.088217
10.	1024.097769	1.345053	-0.017032	0.218908
11.	1025.442822	1.327453	-0.017600	0.187162
12.	1026.770275	1.308557	-0.018896	0.069510
13.	1028.078832	1.290700	-0.017857	0.082756
14.	1029.369532	1.272935	-0.017765	0.087729
15.	1030.642467	1.252566	-0.020369	0.070798
16.	1031.895033	1.233305	-0.019261	0.262768
17.	1033.128338	1.213497	-0.019808	0.299176
18.	1034.341835	1.193768	-0.019729	0.319761
19.	1035.535603	1.174100	-0.019668	0.354873
20.	1036.709703	1.154668	-0.019432	0.392293
21.	1037.864371	1.135671	-0.018997	0.426699
22.	1039.000042	1.116612	-0.019059	0.479641
23.	1040.116654	1.098738	-0.017874	0.309723
24.	1041.215392	1.080896	-0.017842	0.561926
25.	1042.296288	1.061058	-0.019838	0.398465
26.	1043.357346	1.043730	-0.017328	0.655172
27.	1044.401076	1.025638	-0.018092	0.702225
28.	1045.426714	1.007483	-0.018155	0.742763
29.	1046.434197	0.989002	-0.018481	0.776190
30.	1047.423199	0.971565	-0.017437	0.726668
31.	1048.394764	0.953006	-0.018559	0.824693
32.	1049.347770	0.935771	-0.017235	0.857157
33.	1050.283541	0.917274	-0.018497	0.876026
34.	1051.200815	0.899696	-0.017578	0.908528
35.	1052.100511	0.882884	-0.016812	0.932087
36.	1052.983395			0.937363

```
                 (014)E2

    R_branch

 J        wv         delta1      delta2      intens
 2.   1012.694349   1.486708                0.680210
 3.   1014.181057   1.467540   -0.019168   0.904991
 4.   1015.648597   1.447155   -0.020385   0.345968
 5.   1017.095752   1.427168   -0.019987   0.548542
 6.   1018.522920   1.409584   -0.017584   0.411858
 7.   1019.932504   1.391952   -0.017632   0.272203
 8.   1021.324456   1.374249   -0.017703   0.169803
 9.   1022.698705   1.357702   -0.016547   0.072253
10.   1024.056407   1.340562   -0.017140   0.288415
11.   1025.396969   1.322360   -0.018202   0.199055
12.   1026.719329   1.304924   -0.017436   0.314368
13.   1028.024253   1.287283   -0.017641   0.314893
14.   1029.311536   1.269606   -0.017677   0.332851
15.   1030.581142   1.251833   -0.017773   0.340452
16.   1031.832975   1.234022   -0.017811   0.357629
17.   1033.066997   1.216133   -0.017889   0.385023
18.   1034.283130   1.198228   -0.017905   0.409103
19.   1035.481358   1.180184   -0.018044   0.395293
20.   1036.661542   1.160750   -0.019434   0.473103
21.   1037.822292   1.145293   -0.015457   0.256840
22.   1038.967585   1.127156   -0.018137   0.204210
23.   1040.094741   1.110202   -0.016954   0.350686
24.   1041.204943   1.091345   -0.018857   0.435223
25.   1042.296288                           0.398465
```

(021)E1

R branch

J	wv	delta1	delta2	intens
1.	1011.075882	1.495824		0.693858
2.	1012.571706	1.478824	-0.017000	0.550891
3.	1014.050530	1.461824	-0.017000	0.433138
4.	1015.512354	1.444894	-0.016930	0.361661
5.	1016.957248	1.427893	-0.017001	0.313357
6.	1018.385141	1.410832	-0.017061	0.266452
7.	1019.795973	1.392146	-0.018686	0.250349
8.	1021.188119	1.376925	-0.015221	0.167067
9.	1022.565044	1.361281	-0.015644	0.049603
10.	1023.926325	1.343143	-0.018138	0.068123
11.	1025.269468	1.326127	-0.017016	0.064391
12.	1026.595595	1.308970	-0.017157	0.078836
13.	1027.904565	1.291971	-0.016999	0.103115
14.	1029.196536	1.273933	-0.018038	0.143926
15.	1030.470469	1.259070	-0.014863	0.182026
16.	1031.729539	1.237189	-0.021881	0.107564
17.	1032.966728	1.221357	-0.015832	0.103519
18.	1034.188085	1.204592	-0.016765	0.287611
19.	1035.392677	1.186219	-0.018373	0.337873
20.	1036.578896	1.167800	-0.018419	0.383171
21.	1037.746696	1.149676	-0.018124	0.347936
22.	1038.896372	1.130867	-0.018809	0.480176
23.	1040.027239	1.112027	-0.018840	0.519251
24.	1041.139266	1.092687	-0.019340	0.550762
25.	1042.231953	1.073581	-0.019106	0.546533
26.	1043.305534	1.053899	-0.019682	0.636944
27.	1044.359433	1.034559	-0.019340	0.697317
28.	1045.393992	1.013021	-0.021538	0.600252
29.	1046.407013	0.995178	-0.017843	0.709899
30.	1047.402191	0.973561	-0.021617	0.756891
31.	1048.375752	0.953239	-0.020322	0.843145
32.	1049.328991	0.932871	-0.020368	0.824199
33.	1050.261862	0.911737	-0.021134	0.899076
34.	1051.173599	0.890573	-0.021164	0.891542
35.	1052.064172	0.868550	-0.022023	0.895134
36.	1052.932722	0.847979	-0.020571	0.913622

(033)E1

R branch

J	wv	delta1	delta2	intens
2.	1012.748944	1.480766		0.719789
3.	1014.229710	1.462003	-0.018763	0.616200
4.	1015.691713	1.444449	-0.017554	0.546157
5.	1017.136162	1.427496	-0.016953	0.446770
6.	1018.563658	1.410442	-0.017054	0.365976
7.	1019.974100	1.393605	-0.016837	0.310232
8.	1021.367705	1.376207	-0.017398	0.203680
9.	1022.743912	1.359222	-0.016985	0.272751
10.	1024.103134	1.342012	-0.017210	0.265381
11.	1025.445146	1.325129	-0.016883	0.224173
12.	1026.770275	1.308557	-0.016572	0.069510
13.	1028.078832	1.290700	-0.017857	0.082756
14.	1029.369532	1.272935	-0.017765	0.087729
15.	1030.642467	1.256699	-0.016236	0.070798
16.	1031.899166	1.238733	-0.017966	0.291140
17.	1033.137899	1.222231	-0.016502	0.262668
18.	1034.360130	1.204529	-0.017702	0.353921
19.	1035.564659	1.187170	-0.017359	0.398854
20.	1036.751829	1.169750	-0.017420	0.441315
21.	1037.921579	1.152249	-0.017501	0.475486
22.	1039.073828	1.134502	-0.017747	0.510397
23.	1040.208330	1.117610	-0.016892	0.442033
24.	1041.325940	1.099144	-0.018466	0.509980
25.	1042.425084	1.082019	-0.017125	0.645325
26.	1043.507103	1.063241	-0.018778	0.558429
27.	1044.570344	1.045633	-0.017608	0.731079
28.	1045.615977	1.027915	-0.017718	0.708308
29.	1046.643892	1.008887	-0.019028	0.610638
30.	1047.652779	0.988269	-0.020618	0.834284
31.	1048.641048	0.974138	-0.014131	0.861150
32.	1049.615186	0.953629	-0.020509	0.867126
33.	1050.568815	0.934555	-0.019074	0.888392
34.	1051.503370	0.913578	-0.020977	0.850385
35.	1052.416948	0.894799	-0.018779	0.887197
36.	1053.311747	0.866710	-0.028089	0.903860
37.	1054.178457			0.962057

(032)E2

R branch

J	wv	delta1	delta2	intens
2	1012.694349	1.479502		0.680210
3	1014.173851	1.462058	-0.017444	0.501866
4	1015.635909	1.445728	-0.016330	0.424847
5	1017.081637	1.429048	-0.016680	0.347828
6	1018.510685	1.412983	-0.016065	0.286612
7	1019.923668	1.395368	-0.017615	0.118464
8	1021.319036	1.379669	-0.015699	0.236302
9	1022.698705	1.363083	-0.016586	0.072253
10	1024.061788	1.347346	-0.015737	0.181549
11	1025.409134	1.330158	-0.017188	0.093817
12	1026.739292	1.314563	-0.015595	0.213873
13	1028.053855	1.298817	-0.015746	0.138363
14	1029.352672	1.282870	-0.015947	0.248498
15	1030.635542	1.267305	-0.015565	0.237935
16	1031.902847	1.251490	-0.015815	0.162410
17	1033.154337	1.235488	-0.016002	0.299850
18	1034.389825	1.218894	-0.016594	0.335627
19	1035.608719	1.202502	-0.016392	0.338033
20	1036.811221	1.188106	-0.014396	0.188237
21	1037.999327	1.164836	-0.023270	0.298687
22	1039.164163	1.149053	-0.015783	0.487854
23	1040.313216	1.130149	-0.018904	0.502890
24	1041.443365	1.110826	-0.019323	0.574875
25	1042.554191	1.091705	-0.019121	0.592852
26	1043.645896	1.071866	-0.019839	0.661154
27	1044.717762	1.052136	-0.019730	0.721030
28	1045.769898	1.032282	-0.019854	0.749049
29	1046.802180	1.012428	-0.019854	0.781724
30	1047.814608	0.992324	-0.020104	0.810920
31	1048.806932	0.972391	-0.019933	0.856857
32	1049.779323	0.952491	-0.019900	0.870464
33	1050.731814	0.929470	-0.023021	0.895816
34	1051.661284	0.915449	-0.014021	0.877068
35	1052.576733	0.892070	-0.023379	0.932579
36	1053.468803	0.872372	-0.019698	0.937237
37	1054.341175	0.858272	-0.014100	0.937619
38	1055.199447	0.834301	-0.023971	0.879492
39	1056.033748			0.969085

Appendix C

Assignments for the spectrum of CD_3OH in the 910-1300 cm^{-1} region.

C.1 Some of previously assigned series in spreadsheet format.

CD3OH CO-Stretch K=0 A n=0 (010)

CAL @1.00000072

	R Branch					P Branch					Xu R-P	R-P Diff	R-P Diff	Δ(R-P Diff)
J	R(J)	Δ1	Δ2	Int.	J	P(J)	Δ1	Δ2	Int.	J		Calc	R(J)-P(J+2)	Obs - Calc
0	987.12342	1.28931		0.9194	0					0	3.90923	3.90922	3.91002	0.00080
1	988.41273	1.28256	-0.00675	0.8697	1	984.52190	-1.30850		0.8188	1	6.51515	6.51513	6.51516	0.00003
2	989.69529	1.27556	-0.00700	0.8120	2	983.21340	-1.31583	-0.00733	0.7273	2	9.12071	9.12068	9.12066	-0.00002
3	990.97084	1.26849	-0.00706	0.7585	3	981.89757	-1.32295	-0.00712	0.8021	3	11.72578	11.72574	11.72586	0.00012
4	992.23934	1.26123	-0.00726	0.7444	4	980.57463	-1.32964	-0.00669	0.7746	4	14.33021	14.33016	14.33025	0.00009
5	993.50057	1.25368	-0.00756	0.6493	5	979.24499	-1.33590	-0.00626	0.7135	5	16.93387	16.93380	16.93398	0.00018
6	994.75425	1.24617	-0.00751	0.6712	6	977.90909	-1.34250	-0.00660	0.6579	6	19.53660	19.53651	19.53662	0.00011
7	996.00041	1.23836	-0.00780	0.6355	7	976.56659	-1.34896	-0.00646	0.6843	7	22.13829	22.13816	22.13834	0.00018
8	997.23878	1.23043	-0.00793	0.6148	8	975.21763	-1.35555	-0.00660	0.6614	8	24.73877	24.73860	24.73882	0.00022
9	998.46921	1.22221	-0.00822	0.5887	9	973.86208	-1.36212	-0.00657	0.6467	9	27.33792	27.33770	27.33801	0.00031
10	999.69143	1.21398	-0.00824	0.6083	10	972.49996	-1.36875	-0.00663	0.6386	10	29.93561	29.93530	29.93563	0.00033
11	1000.90541	1.20526	-0.00872	0.5781	11	971.13121	-1.37541	-0.00666	0.6278	11	32.53170	32.53127	32.53173	0.00046
12	1002.11067	1.19678	-0.00848	0.5928	12	969.75580	-1.38212	-0.00671	0.6102	12	35.12606	35.12547	35.12597	0.00050
13	1003.30745	1.18782	-0.00896	0.5930	13	968.37368	-1.38898	-0.00686	0.6146	13	37.71858	37.71775	37.71862	0.00087
14	1004.49527	1.17825	-0.00956	0.5618	14	966.98470	-1.39587	-0.00689	0.6371	14	40.30912	40.30797	40.30929	0.00132
15	1005.67352	1.16949	-0.00876	0.5847	15	965.58883	-1.40285	-0.00698	0.6402	15	42.89758	42.89599	42.89746	0.00147
16	1006.84301	1.15989	-0.00960	0.6109	16	964.18598	-1.40992	-0.00706	0.6382	16	45.48386	45.48167	45.48408	0.00241
17	1008.00290	1.14962	-0.01028	0.5817	17	962.77606	-1.41713	-0.00722	0.6577	17	48.06785	48.06487	48.06819	0.00332
18	1009.15252	1.13940	-0.01021	0.6532	18	961.35893	-1.42421	-0.00708	0.6760	18	50.64947	50.64543	50.64977	0.00434
19	1010.29193	1.13058	-0.00882	0.5438	19	959.93472	-1.43197	-0.00776	0.6310	19	53.22865	53.22323	53.22831	0.00508
20	1011.42251	1.11952	-0.01106	0.6816	20	958.50275	-1.43914	-0.00717	0.7053	20	55.80532	55.79812	55.80559	0.00747
21	1012.54203	1.10950	-0.01001	0.3883	21	957.06361	-1.44669	-0.00756	0.5789	21	58.37942	58.36996	58.37965	0.00969
22	1013.65153	1.09963	-0.00987	0.5387	22	955.61692	-1.45454	-0.00785	0.7116	22	60.95091	60.93860	60.95161	0.01301
23	1014.75116	1.08858	-0.01105	0.7337	23	954.16238	-1.46246	-0.00791	0.6642	23	63.51977	63.50391	63.52109	0.01718
24	1015.83974	1.07835	-0.01023	0.7671	24	952.69992	-1.46986	-0.00740	0.7445	24	66.08598	66.06574	66.08744	0.02170
25	1016.91810	1.06774	-0.01062	0.8027	25	951.23007	-1.47777	-0.00791	0.8020	25		68.62394	68.65176	0.02782
26	1017.98583	1.05763	-0.01011	0.8177	26	949.75230	-1.48596	-0.00819	0.8169	26		71.17839	71.21262	0.03423
27	1019.04346	1.04723	-0.01040	0.8584	27	948.26634	-1.49313	-0.00717	0.8397	27		73.72893	73.77107	0.04214
28	1020.09069	1.03685	-0.01038	0.8618	28	946.77321	-1.50082	-0.00770	0.8165	28		76.27543	76.32706	0.05163
29	1021.12754	1.02665	-0.01020	0.8761	29	945.27239	-1.50876	-0.00794	0.8314	29		78.81773	78.88081	0.06308
30	1022.15419	1.01702	-0.00963	0.8843	30	943.76363	-1.51690	-0.00814	0.6574	30		81.35571	81.43216	0.07645
31	1023.17121	1.00688	-0.01014	0.9037	31	942.24673	-1.52470	-0.00780	0.8778	31		83.88922	#########	939.28199
32	1024.17809	0.99732	-0.00957	0.9101	32	940.72203	-940.72203	-939.19733	0.9160	32		86.41811	#########	937.76998
33	1025.17541	0.98746	-0.00986	0.9168						33		88.94224	#########	936.23317
34	1026.16287	0.97926	-0.00821	0.9251						34		91.46148	#########	934.70139
35	1027.14213	-1027.14213	-1028.12138	0.9355						35		93.97568		-93.97568
36		0.00000	1027.14213							36				
		0.00000	0.00000											

CD3OH CO-Stretch K=0 E n=0 (030)

CAL@1.00000072

	R Branch					P Branch					Xu R-P	R-P Diff	R-P Diff	Δ(R-P Diff)
J	R(J)	Δ1	Δ2	Int.	J	P(J)	Δ1	Δ2	Int.	J		Calc	R(J)-P(J+2)	Obs - Calc
0	986.82000	1.27151		0.9067						0	3.90550	3.90513	3.90542	0.00029
1	988.09150	1.26007	-0.01143	0.8598*Bc	1	984.23138	-1.31680		0.8800?	1	6.49815	6.49355	6.49915	0.00560
2	989.35158	1.25510	-0.00498	0.8281	2	982.91458	-1.32222	-0.00543	0.8108	2	9.08336	9.05949	9.08302	0.02353
3	990.60668	1.25062	-0.00448	0.7554	3	981.59236	-1.32380	-0.00158	0.7721	3	11.66744	11.59396	11.66748	0.07352
4	991.85729	1.24481	-0.00581	0.6806	4	980.26856	-1.32936	-0.00556	0.6421	4	14.25305	14.08795	14.25307	0.16512
5	993.10210	1.23782	-0.00699	0.6261*	5	978.93919	-1.33497	-0.00561	0.6593	5	16.83958	16.53247	16.83960	0.30713
6	994.33992	1.23013	-0.00769	0.5544	6	977.60422	-1.34172	-0.00675	0.6181	6	19.42611	18.91853	19.42614	0.50761
7	995.57005	1.22189	-0.00824	0.5488	7	976.26250	-1.34872	-0.00700	0.5853	7	22.01209	21.23714	22.01210	0.77496
8	996.79194	1.21348	-0.00841	0.5186	8	974.91377	-1.35583	-0.00711	0.5541	8	24.59721	23.47930	24.59723	1.11793
9	998.00542	1.20485	-0.00864	0.5048	9	973.55794	-1.36323	-0.00740	0.5356	9	27.18127	25.63602	27.18129	1.54527
10	999.21027	1.19598	-0.00887	0.4942	10	972.19471	-1.37057	-0.00734	0.5359	10	29.76414	27.69830	29.76427	2.06597
11	1000.40624	1.18700	-0.00898	0.4795	11	970.82413	-1.37813	-0.00756	0.5233	11	32.34574	29.65715	32.34576	2.68861
12	1001.59324	1.17813	-0.00887	0.4366	12	969.44600	-1.38551	-0.00738	.2610G*B	12	34.92600	31.50358	34.92604	3.42246
13	1002.77137	1.16903	-0.00910	0.4958	13	968.06049	-1.39329	-0.00778	0.5031	13	37.50487	33.22858	37.50496	4.27638
14	1003.94040	1.15993	-0.00910	0.4969	14	966.66720	-1.40078	-0.00750	0.5192	14	40.08234	34.82318	40.08268	5.25950
15	1005.10032	1.15070	-0.00923	0.5051	15	965.26641	-1.40870	-0.00791	0.5381	15	42.65838	36.27837	42.65859	6.38022
16	1006.25102	1.14174	-0.00896	0.4688	16	963.85772	-1.41599	-0.00729	0.3170*	16	45.23299		45.23310	45.23310
17	1007.39276	1.13276	-0.00898	0.5199	17	962.44173	-1.42381	-0.00782	0.5359	17	47.80617		47.80631	47.80631
18	1008.52552	1.12361	-0.00915	0.5634	18	961.01792	-1.43147	-0.00767	0.5792	18	50.37791		50.37813	50.37813
19	1009.64914	1.11474	-0.00887	0.5824	19	959.58645	-1.43906	-0.00759	0.5974	19	52.94822		52.94856	52.94856
20	1010.76388	1.10601	-0.00873	0.5831	20	958.14739	-1.44682	-0.00776	0.5123*	20	55.51711		55.51765	55.51765
21	1011.86989	1.09784	-0.00817	0.6272	21	956.70057	-1.45434	-0.00753	0.6418	21	58.08458		58.08519	58.08519
22	1012.96773	1.08867	-0.00916	0.5490*Bc	22	955.24623	-1.46153	-0.00719	0.6613	22	60.65061		60.65173	60.65173
23	1014.05640	1.08344	-0.00524	0.6386	23	953.78470	-1.46870	-0.00717	0.6558	23	63.21521		63.21589	63.21589
24	1015.13984	1.07838	-0.00505	0.7143	24	952.31600	-1.47549	-0.00679	.7187G*B	24	65.77836		65.77968	65.77968
25	1016.21822	1.08320	0.00482	0.7995	25	950.84051	-1.48035	-0.00486	0.7156	25			68.34281	68.34281
26	1017.30142	-1017.30142	-1018.38462	0.7479	26	949.36016	-1.48475	-0.00440	0.7701	26			70.92702	70.92702
27		0.00000	1017.30142		27	947.87541	-1.50101	-0.01625	0.7536*	27			0.00000	0.00000
28		0.00000	0.00000		28	946.37440	-946.37440	-944.87339	0.8534	28			0.00000	0.00000
29		0.00000	0.00000		29		0.00000	946.37440		29			0.00000	0.00000
30		0.00000	0.00000		30		0.00000	0.00000		30			0.00000	0.00000
31		0.00000	0.00000		31		0.00000	0.00000		31			0.00000	0.00000
32		0.00000	0.00000		32					32			0.00000	0.00000
33		0.00000	0.00000							33			0.00000	0.00000
34		0.00000	0.00000							34			0.00000	0.00000
35		0.00000	0.00000							35				0.00000
36		0.00000	0.00000							36				
		0.00000	0.00000											

CD3OH CO-Stretch K=1 E1 n=1 (121)															
Cal● 1.00000072															
	R Branch					P Branch					Calc Q	Q Branch			
J	R(J)	Δ1	Δ2	Int.	J	P(J)	Δ1	Δ2	Int.	J	P	Q(J)	Δ1	Δ2	Int.
1	987.76130	1.27835		0.9249	1					1	2.60004	985.18016	-0.01583		0.4597
2	989.03965	1.27078	-0.00757	0.8924	2		981.26121			2	985.16110	985.16433	-0.02253	-0.00670	0.4822
3	990.31043	1.26361	-0.00717	0.8698	3	981.26121	-1.32090	-982.58211	0.8968	3	985.13983	985.14160	-0.02970	-0.00717	0.7094
4	991.57404	1.25607	-0.00754	0.8411	4	979.94031	-1.32857	-0.00767	0.8232	4	985.11096	985.11210	-0.03593	-0.00623	0.3880
5	992.83011	1.24884	-0.00723	0.8146	5	978.61174	-1.33585	-0.00728	0.8436	5	985.07471	985.07617	-0.04186	-0.00593	0.6414
6	994.07895	1.24136	-0.00748	0.7999	6	977.27589	-1.34287	-0.00702	0.8197	6	985.03120	985.03431	-0.05194	-0.01008	0.6572
7	995.32031	1.23406	-0.00730	0.7619	7	975.93302	-1.34962	-0.00675	7975/10R	7	984.98075	984.98237	-0.05989	-0.00795	0.4374
8	996.55437	1.22613	-0.00793	0.7595	8	974.58340	-1.35687	-0.00725	0.7916	8	984.92285	984.92248	-0.06428	-0.00439	0.4882
9	997.78050	1.21971	-0.00642	0.6137	9	973.22653	-1.36357	-0.00670	0.7861	9	984.85801	984.85820	-0.05990	0.00438	0.7610
10	999.00021	1.21194	-0.00777	0.7466	10	971.86296	-1.37116	-0.00759	0.7459	10	984.78530	984.79830	-0.08819	-0.02829	0.6560
11	1000.21215	1.20449	-0.00745	0.7398	11	970.49180	-1.37679	-0.00563	0.5913	11	984.70666	984.71011	-0.08685	0.00134	0.5822
12	1001.41664	1.19745	-0.00704	0.7326	12	969.11501	-1.38414	-0.00735	0.7271	12	984.62034	984.62326	-0.09456	-0.00771	0.8620
13	1002.61409	1.18935	-0.00810	0.6814	13	967.73087	-1.39070	-0.00656	0.7292	13	984.52713	984.52870	-0.10144	-0.00688	0.8925
14	1003.80344	1.18233	-0.00702	0.7315	14	966.34017	-1.39735	-0.00665	0.7639	14	984.42687	984.42726	-0.10511	-0.00367	0.8077
15	1004.98577	1.17499	-0.00734	0.7433	15	964.94282	-1.40418	-0.00683	0.7664	15	984.31924	984.32215	-0.11677	-0.01166	0.7893
16	1006.16076	1.16763	-0.00736	0.7463	16	963.53864	-1.41032	-0.00614	0.7355	16	984.20509	984.20538	-0.12174	-0.00497	0.8730
17	1007.32839	1.16025	-0.00738	0.7382	17	962.12832	-1.41704	-0.00672	0.7807	17	984.08396	984.08364	-0.12243	-0.00069	0.8070
18	1008.48864	1.15300	-0.00725	0.7737	18	960.71128	-1.42399	-0.00695	0.7922	18	983.95519	983.96121	-0.13359	-0.01116	0.8544
19	1009.64164	1.14567	-0.00733	0.7864	19	959.28729	-1.42894	-0.00495	0.7385	19	983.82077	983.82762	-0.14509	-0.01150	0.8278
20	1010.78731	1.13835	-0.00732	0.8076	20	957.85835	-1.43590	-0.00696	0.6761	20	983.67896	983.68253	-0.14402	0.00107	0.7829
21	1011.92566	1.13244	-0.00591	0.7812	21	956.42245	-1.44177	-0.00587	0.6987	21	983.53062	983.53851	-0.15672	-0.01270	0.7702
22	1013.05810	1.12234	-0.01010	0.8120	22	954.98068	-1.44796	-0.00619	0.7467	22	983.37577	983.38179	-0.16395	-0.00723	0.8291
23	1014.18044	1.11681	-0.00553	0.8167	23	953.53272	-1.45369	-0.00573	0.7813	23	983.21433	983.21784	-0.16967	-0.00572	0.8137
24	1015.29725	1.10999	-0.00682	0.7402	24	952.07903	-1.46047	-0.00678	0.7852	24	983.04526	983.04817	-0.17200	-0.00233	0.8357
25	1016.40724	1.10234	-0.00765	0.8824	25	950.61856	-1.46601	-0.00554	0.8416	25	982.87039	982.87617	-0.18293	-0.01093	0.9106
26	1017.50958	1.09537	-0.00697	0.8522	26	949.15255	-1.47175	-0.00574	0.8572	26	982.68910	982.69324	-0.15636	0.02657	0.7274
27	1018.60495	1.08827	-0.00710	0.9169	27	947.68080	-1.47774	-0.00599	0.8552	27	982.50097	982.53688	-0.22569	-0.06933	0.9404
28	1019.69322	1.08137	-0.00690	0.9023	28	946.20306	-1.48299	-0.00525	0.8649	28	982.30683	982.31119	-0.19800	0.02769	0.8856
29	1020.77459	1.07442	-0.00695	0.9244	29	944.72007	-1.48875	-0.00576	0.8844	29		982.11319	-0.14961	0.04839	0.9209
30	1021.84901	1.06891	-0.00551	0.9266	30	943.23132	-1.49406	-0.00531	0.8873	30		981.96358	-0.26532	-0.11571	0.9297
31	1022.91792	1.05963	-0.00928	0.9142	31	941.73726	-1.49944	-0.00538	0.8996	31		981.69826	-0.22787	0.03745	0.8833
32	1023.97755	-1023.97755	-1025.03718	0.9524	32	940.23782	-1.50487	-0.00543	0.9265	32		981.47039	-0.22651	0.00136	0.9377
33		0.00000	1023.97755		33	938.73295	-938.73295	-937.22808	0.9190	33		981.24388	-0.23252	-0.00601	0.8955
34										34		981.01136	-0.24333	-0.01081	0.9265
35										35		980.76803	-0.09484	0.14849	0.9370
36										36		980.67319	-0.26937	-0.17453	0.8949
										37		980.40382	-0.28028	-0.01091	0.8728
										38		980.12354	-0.25626	0.02402	0.8940
										39		979.86728	-0.27745	-0.02119	0.9444
										40		979.58983	-979.58983	-979.31238	0.8868

	R-P Diff	R-P Diff				Calc a-Type
J	Calc	Obs	Obs-Calc	Δ1	Δ2	Gd
1	6.49966	6.50009	0.00043			2.60004
2	9.09933	9.09934	0.00001	-0.00042	0.00030	3.89989
3	11.69880	11.69869	-0.00011	-0.00012	0.00036	5.19952
4	14.29802	14.29815	0.00013	0.00024	-0.00022	6.49922
5	16.89694	16.89709	0.00015	0.00002	-0.00011	7.79882
6	19.49549	19.49555	0.00006	-0.00009	0.00019	9.09818
7	22.09362	22.09378	0.00016	0.00010	-0.00013	10.39735
8	24.69128	24.69141	0.00013	-0.00003	0.00019	11.69632
9	27.28841	27.28870	0.00029	0.00016	-0.00021	12.99505
10	29.88496	29.88520	0.00024	-0.00005	0.00023	14.29350
11	32.48086	32.48128	0.00042	0.00018		15.59165
12	35.07607	35.07647	0.00040			16.88947
13		37.67127	37.67127			18.18696
14		40.26480	40.26480			19.48405
15		42.85745	42.85745			20.78060
16		45.44948	45.44948			22.07677
17		48.04110	48.04110			23.37268
18		50.63029	50.63029			24.66790
19		53.21919				25.96242
20		55.80663				27.25651
21		58.39294				28.54994
22		60.97907				29.84305
23		63.56188				31.13530
24		66.14470				32.42670
25		68.72644				33.71784
26		71.30652				35.00830
27		73.88488				36.29791
28		76.46190				37.58676
29		79.03733				
30		81.61119				
31		84.18497				
32		1023.97755				
33		0.00000				
34		0.00000				
35		0.00000				
36		0.00000				
37		0.00000				
38						
39						
40						

CD3OH CO-Stretch K=4 E1 n=1 (124)															
	R Branch					P Branch					Calc Q	Q Branch			
J	R(J)	Δ1	Δ2	Int.	J	P(J)	Δ1	Δ2	Int.	J	P	Q(J)	Δ1	Δ2	Int.
4	991.43386	1.25429		0.9382	4					4	984.97313	984.97224	-0.03624		0.6148
5	992.68815	1.24669	-0.00760	0.7404	5	978.47464	-1.33746		0.9272/10R	5	984.93508	984.93600	-0.04627	-0.01003	0.5829
6	993.93484	1.23892	-0.00777	0.7224	6	977.13718	-1.34385	-0.00639	0.8568	6	984.89032	984.88973	-0.05213	-0.00586	0.5069
7	995.17376	1.23194	-0.00758	0.8139	7	975.79333	-1.35155	-0.00770	0.8632	7	984.83779	984.83760	-0.05769	-0.00556	0.8106
8	996.40510	1.22373	-0.00761	0.8093	8	974.44178	-1.35891	-0.00736	0.8391	8	984.77769	984.77991	-0.06980	-0.01211	0.7432
9	997.62883	1.21602	-0.00771	0.7945	9	973.08287	-1.36609	-0.00718	0.8014	9	984.71021	984.71011	-0.07446	-0.00466	0.5822
10	998.84485	1.20834	-0.00768	0.7627	10	971.71678	-1.37325	-0.00716	0.8019	10	984.63526	984.63565	-0.08000	-0.00554	0.8000
11	1000.05319	1.20068	-0.00766	0.7568	11	970.34353	-1.38018	-0.00693	0.7996	11	984.55294	984.55565	-0.09138	-0.01138	0.6871
12	1001.25387	1.19297	-0.00771	0.7745	12	968.96335	-1.38688	-0.00670	0.7920	12	984.46368	984.46427	-0.09765	-0.00627	0.7055
13	1002.44684	1.18550	-0.00747	0.7754	13	967.57647	-1.39463	-0.00775	0.7048	13	984.36650	984.36662	-0.09993	-0.00228	0.6272
14	1003.63234	1.17778	-0.00772	0.7624	14	966.18184	-1.40150	-0.00687	0.7062	14	984.26201	984.26669	-0.11603	-0.01610	0.8174
15	1004.81012	1.17036	-0.00742	0.7553	15	964.78034	-1.40803	-0.00653	0.7709	15	984.15051	984.15066	-0.11967	-0.00364	0.8943
16	1005.98048	1.16353	-0.00683	0.7598	16	963.37231	-1.41482	-0.00679	0.7983	16	984.03180	984.03099	-0.12400	-0.00433	0.7927
17	1007.14401	1.15494	-0.00859	0.7224	17	961.95749	-1.42147	-0.00665	0.7978	17	983.90616	983.90699	-0.13170	-0.00770	0.8648
18	1008.29895	1.14887	-0.00607	0.7769	18	960.53602	-1.42796	-0.00649	0.8079	18	983.77345	983.77529	-983.77529	-983.64359	0.6987
19	1009.44782	1.14267	-0.00620	0.7985	19	959.10806	-1.43455	-0.00659	0.7166	19	983.63347		0.00000	983.77529	
20	1010.59049	1.13865	-0.00402	0.6495	20	957.67351	-1.43992	-0.00537	0.8150	20	1216.63372		0.00000	0.00000	
21	1011.72914	-1011.72914	-1012.86779	0.8170	21	956.23359	-956.23359	-954.79367	0.8337	21	505.83472		0.00000	0.00000	
22		0.00000	1011.72914		22		0.00000	956.23359		22	258.55300		0.00000	0.00000	
23		0.00000	0.00000		23		0.00000	0.00000		23	0.00000		0.00000	0.00000	
24		0.00000	0.00000		24		0.00000	0.00000		24	0.00000		0.00000	0.00000	
25					25					25	0.00000		0.00000	0.00000	
26					26					26	0.00000		0.00000	0.00000	
27					27					27	0.00000		0.00000	0.00000	
28					28					28	0.00000		0.00000	0.00000	
29					29					29	0.00000		0.00000	0.00000	
30					30					30	0.00000		0.00000	0.00000	
31					31					31	0.00000		0.00000	0.00000	
32					32					32			0.00000	0.00000	
33										33			0.00000	0.00000	
34										34			0.00000	0.00000	
35										35					
36										36					
										37					
										38					
										39					
										40					

	R-P Diff	R-P Diff				Calc a-Type
J	Calc	Obs	Obs-Calc	Δ1	Δ2	Gd
4	14.29605	14.29668	0.00063			6.49849
5	16.89462	16.89482	0.00020	-0.00043	0.00045	7.79790
6	19.49284	19.49306	0.00022	0.00002	-0.00001	9.09699
7	22.09066	22.09089	0.00023	0.00001	0.00006	10.39601
8	24.68802	24.68832	0.00030	0.00007	0.00007	11.69482
9	27.28486	27.28530	0.00044	0.00014	-0.00020	12.99343
10	29.88112	29.88150	0.00038	-0.00006	-0.00037	14.29173
11	32.47677	32.47672	-0.00005	-0.00043	0.00077	15.58959
12	35.07174	35.07203	0.00029	0.00034	-0.00010	16.88721
13	37.66597	37.66650	0.00053	0.00024	-0.00016	18.18466
14	40.25942	40.26003	0.00061	0.00008	-0.00009	19.48167
15	42.85203	42.85263	0.00060	-0.00001	45.44387	20.77820
16		45.44446	45.44446	45.44386	-45.44386	22.07431
17		48.03595	48.03595			23.37014
18		50.62544	50.62544			24.66539
19		53.21423	53.21423			25.95996
20		1010.59049	1010.59049			260.40013
21		1011.72914	1011.72914			505.83472
22		0.00000				258.55300
23		0.00000				0.00000
24		0.00000				0.00000
25		0.00000				0.00000
26		0.00000				0.00000
27		0.00000				0.00000
28		0.00000				0.00000
29		0.00000				0.00000
30		0.00000				0.00000
31		0.00000				0.00000
32		0.00000				
33		0.00000				
34		0.00000				
35		0.00000				
36		0.00000				
37		0.00000				
38		0.00000				
39		0.00000				
40		0.00000				

CD3OH CO-Stretch K=5 A n=1 (125)															
	R Branch					P Branch					Calc Q	Q Branch			
J	R(J)	Δ1	Δ2	Int.	J	P(J)	Δ1	Δ2	Int.	J	P	Q(J)	Δ1	Δ2	Int.
5	992.66624	1.22848		0.9081	5					5	984.93396	984.93173	-0.06247		0.2734
6	993.89472	1.22078	-0.00770	0.8653	6	977.13718	-1.36397		0.8568	6	984.86934	984.86926	-0.07063	-0.00816	0.4364
7	995.11550	1.21364	-0.00714	0.8420	7	975.77321	-1.36994	-0.00597	0.8427	7	984.79835	984.79863	-0.07897	-0.00834	0.6560
8	996.32914	1.20752	-0.00612	0.6260	8	974.40327	-1.37657	-0.00663	0.8189	8	984.72034	984.71966	-0.08401	-0.00504	0.7430
9	997.53666	1.19988	-0.00764	0.7827	9	973.02670	-1.38323	-0.00666	0.8348	9	984.63561	984.63565	-0.09089	-0.00688	0.8000
10	998.73654	1.19284	-0.00704	0.7765	10	971.64347	-1.38965	-0.00642	0.8167	10	984.54426	984.54476	-0.09868	-0.00779	0.5897
11	999.92938	1.18570	-0.00714	0.7896	11	970.25382	-1.39609	-0.00644	0.7453	11	984.44605	984.44608	-0.10536	-0.00668	0.7080
12	1001.11508	1.17864	-0.00706	0.7736	12	968.85773	-1.40270	-0.00661	0.8081	12	984.34092	984.34072	-0.10934	-0.00398	0.7285
13	1002.29372	1.17145	-0.00719	0.7574	13	967.45503	-1.40905	-0.00635	0.7985	13	984.22910	984.23138	-0.11917	-0.00983	0.8800
14	1003.46517	1.16438	-0.00707	0.7375	14	966.04598	-1.41552	-0.00647	0.8031	14	984.11046	984.11221	-0.12726	-0.00809	0.8164
15	1004.62955	1.15729	-0.00709	0.7687	15	964.63046	-1.42190	-0.00638	0.8117	15	983.98504	983.98495	-0.13185	-0.00459	0.6469
16	1005.78684	1.15015	-0.00714	0.7836	16	963.20856	-1.42817	-0.00627	0.8222	16	983.85287	983.85310	-0.13802	-0.00617	0.9269
17	1006.93699	1.14153	-0.00862	0.7490	17	961.78039	-1.43416	-0.00599	0.7994	17	983.71417	983.71508	-0.14225	-0.00423	0.8680
18	1008.07852	1.13869	-0.00284	0.6006	18	960.34623	-1.44023	-0.00607	0.8215	18	983.56854	983.57283	-0.15114	-0.00889	0.7641
19	1009.21721	1.12876	-0.00993	0.7238	19	958.90600	-1.44643	-0.00620	ch	19	983.41687	983.42169	-0.15870	-0.00756	0.8809
20	1010.34597	1.12262	-0.00614	0.6561	20	957.45957	-1.45250	-0.00607	0.8412	20	983.25893	983.26299	-0.16377	-0.00507	9221/10R
21	1011.46859	1.11267	-0.00995	0.6685	21	956.00707	-1.45818	-0.00568	0.8562	21	983.09415	983.09922	-0.14196	0.02181	0.8186
22	1012.58126	1.10246	-0.01021	0.6588	22	954.54889	-1.46409	-0.00591	8535/10R	22	982.92240	982.95726	-0.19148	-0.04952	0.9047
23	1013.68372	1.08747	-0.01499	0.5255	23	953.08480	-1.46987	-0.00578	0.8797	23	982.74263	982.76578	-0.21013	-0.01865	0.8918
24	1014.77119	-1014.77119	-1015.85866	0.6874	24	951.61493	-1.47535	-0.00548	0.8875	24	982.55392	982.55565	-0.19559	0.01454	0.8625
25					25	950.13958	-1.48110	-0.00575	0.9007	25	733.18556	982.36006	-0.20341	-0.00782	0.9228
26					26	948.65848	-1.48659	-0.00549	0.9087	26	473.78973	982.15665	-0.19307	0.01034	0.8299
27					27	947.17189	-1.49214	-0.00555	0.9245	27	473.05681	981.96358	-0.30035	-0.10728	0.9297
28					28	945.67975	-1.49731	-0.00517	0.9293	28	703.99568	981.66323	-0.27767	0.02268	0.9073
29					29	944.18244	-944.18244	-942.68513	0.9212	29	0.00000	981.38556	-0.23505	0.04262	0.8104
30					30					30	0.00000	981.15051	-0.38656	-0.15151	0.8212
31					31					31	0.00000	980.76395	-0.32621	0.06035	0.9328
32					32					32	0.00000	980.43774	-0.39157	-0.06536	0.9089
33										33		980.04617	-0.45634	-0.06477	0.7793
34										34		979.58983	-0.35240	0.10394	0.8868
35										35		979.23743	6.89067	7.24307	0.9225
36										36		986.12810	-0.70019	-7.59086	0.9475
										37		985.42791	-0.68131	0.01888	0.2934
										38		984.74660	-0.76165	-0.08034	0.8911
										39		983.98495	-0.86060	-0.09895	0.6469
										40		983.12435	-983.12435	-982.26375	0.8348

	Xu R-P	R-P Diff	R-P Diff					Calc a-Type	Calc a-Type
J		Calc	Obs	Obs-Calc	Δ1	Δ2	J	Gd	Exc
5	16.89327	16.89307	16.89303	-0.00004			5	7.79678	7.73425
6	19.49130	19.49106	19.49145	0.00039	0.00043	-0.00066	6	9.09613	9.02485
7	22.08892	22.08864	22.08880	0.00016	-0.00023	-0.00002	7	10.39508	10.31697
8	24.68609	24.68576	24.68567	-0.00009	-0.00025	0.00081	8	11.69364	11.60890
9	27.28274	27.28237	27.28284	0.00047	0.00056	-0.00063	9	12.99214	12.90072
10	29.87883	29.87841	29.87881	0.00040	-0.00007	0.00020	10	14.29044	14.19213
11	32.47430	32.47382	32.47435	0.00053	0.00013	-0.00012	11	15.58832	15.48321
12	35.06910	35.06856	35.06910	0.00054	0.00001	0.00014	12	16.88589	16.77400
13	37.66317	37.66257	37.66326	0.00069	0.00015	-0.00003	13	18.18312	18.06447
14	40.25645	40.25580	40.25661	0.00081	0.00012	0.00004	14	19.48000	19.35458
15	42.84869	42.84819	42.84916	0.00097	0.00016	-0.00020	15	20.77648	20.64435
16	45.44045	45.43968	45.44061	0.00093	-0.00004	48.03010	16	22.07248	21.93374
17	48.03105		48.03099	48.03099	48.03006	-48.03006	17	23.36794	23.22225
18	50.62064		50.61895	50.61895			18	24.66254	24.51088
19	53.20916		53.21014	53.21014			19	25.95730	25.79943
20	55.79660		55.79708	55.79708			20	27.25186	27.08701
21	58.38284		58.38379	58.38379			21	28.54526	28.37352
22	60.96785		60.96633	60.96633			22	29.83760	29.65789
23	63.55158		63.54414				23	31.12770	30.93890
24	66.13396		66.11271				24	32.41434	-216.76606
25			-947.17189				25	-215.47292	-474.88226
26			-945.67975				26	-473.36216	-474.12707
27			-944.18244				27	-472.62294	-473.37052
28			0.00000				28	-240.18676	-472.61249
29			0.00000				29	0.00000	-240.04638
30			0.00000				30	0.00000	0.00000
31			0.00000				31	0.00000	0.00000
32			0.00000				32	0.00000	0.00000
33			0.00000				33		
34			0.00000				34		
35			0.00000				35		
36			0.00000				36		
37			0.00000				37		
38			0.00000				38		
39			0.00000				39		
40			0.00000				40		
			0.00000						

CD3OH CO-Stretch K=0 E1 n=1 (130)

	R Branch					P Branch					R-P Diff	R-P Diff	
J	R(J)	Δ1	Δ2	Int.	J	P(J)	Δ1	Δ2	Int.	J	Calc	Obs	Obs-Calc
0	986.37470	1.28534		0.9586	0					0	3.89986	3.90003	0.00017
1	987.66004	1.27811	-0.00723	0.9198	1	983.78144	-1.30677		0.8843	1	6.49967	6.49962	-0.00005
2	988.93815	1.27116	-0.00695	0.8814	2	982.47467	-1.31425	-0.00748	0.8909	2	9.09933	9.09869	-0.00064
3	990.20931	1.26321	-0.00795	0.8077	3	981.16042	-1.32096	-0.00671	0.8847	3	11.69880	11.69862	-0.00018
4	991.47252	1.25691	-0.00630	0.7956	4	979.83946	-1.32877	-0.00781	0.8220	4	14.29802	14.29783	-0.00019
5	992.72943	1.24891	-0.00800	0.7969	5	978.51069	-1.33600	-0.00723	0.7569	5	16.89692	16.89701	0.00009
6	993.97834	1.24171	-0.00720	0.7703	6	977.17469	-1.34227	-0.00627	0.6929	6	19.49545	19.49554	0.00009
7	995.22005	1.23428	-0.00743	0.7666	7	975.83242	-1.34962	-0.00735	0.7880	7	22.09355	22.09365	0.00010
8	996.45433	1.22692	-0.00736	0.7292	8	974.48280	-1.35640	-0.00678	0.7767	8	24.69117	24.69132	0.00015
9	997.68125	1.21856	-0.00836	0.7229	9	973.12640	-1.36339	-0.00699	0.7672	9	27.28825	27.28855	0.00030
10	998.89981	1.21273	-0.00583	0.6621	10	971.76301	-1.37031	-0.00692	0.7641	10	29.88473	29.88417	-0.00056
11	1000.11254	1.20458	-0.00815	0.7392	11	970.39270	-1.37706	-0.00675	0.6906	11	32.48055	32.48079	0.00024
12	1001.31712	1.19718	-0.00740	0.7349	12	969.01564	-1.38389	-0.00683	0.7602	12	35.07567	35.07582	0.00015
13	1002.51430	1.18964	-0.00754	0.7299	13	967.63175	-1.39045	-0.00656	0.7613	13		37.67050	37.67050
14	1003.70394	1.18206	-0.00758	0.7392	14	966.24130	-1.39750	-0.00705	0.5393	14		40.26404	40.26404
15	1004.88600	1.17463	-0.00743	0.7357	15	964.84380	-1.40390	-0.00640	0.7533	15		42.85678	42.85678
16	1006.06063	1.16715	-0.00748	0.7548	16	963.43990	-1.41068	-0.00678	0.7726	16		45.44812	45.44812
17	1007.22778	1.15971	-0.00744	0.7567	17	962.02922	-1.41671	-0.00603	0.7515	17		48.03940	48.03940
18	1008.38749	1.15225	-0.00746	0.7760	18	960.61251	-1.42413	-0.00742	0.7687	18		50.62918	
19	1009.53974	1.14447	-0.00778	0.7985	19	959.18838	-1.43007	-0.00594	0.8108	19		53.21815	
20	1010.68421	1.13695	-0.00752	0.8091	20	957.75831	-1.43672	-0.00665	0.8146	20		55.80548	
21	1011.82116	1.12953	-0.00742	0.8104	21	956.32159	-1.44286	-0.00614	0.8062	21		58.39174	
22	1012.95069	1.12198	-0.00755	0.8049	22	954.87873	-1.44931	-0.00645	0.8424	22		60.97684	
23	1014.07267	1.11458	-0.00740	0.8445	23	953.42942	-1.45557	-0.00626	0.8483	23		63.56058	
24	1015.18725	1.10769	-0.00689	0.8689	24	951.97385	-1.46176	-0.00619	0.8646	24		66.14330	
25	1016.29494	1.09869	-0.00900	0.8238	25	950.51209	-1.46814	-0.00638	0.8803	25		68.72492	
26	1017.39363	1.09181	-0.00688	0.8355	26	949.04395	-1.47393	-0.00579	0.8915	26		71.30359	
27	1018.48544	1.08408	-0.00773	0.9086	27	947.57002	-1.47998	-0.00605	0.8996	27		73.88228	
28	1019.56952	1.07387	-0.01021	0.9014	28	946.09004	-1.48688	-0.00690	0.8954	28		76.45821	
29	1020.64339	1.07133	-0.00254	.8706*	29	944.60316	-1.49185	-0.00497	0.8899	29		1020.64339	
30	1021.71472	-1021.71472	-1022.78605	.9127*	30	943.11131	-943.11131	-941.61946	0.9097	30		1021.71472	
31					31					31		0.00000	
32					32					32		0.00000	
33										33		0.00000	
34										34		0.00000	
35										35		0.00000	
36										36		0.00000	
										37			

CO3OH CO-Stretch K=1 A± n=1 (131)																	
	R Branch					R Branch					P Branch					P Branch	
J	R(J) A+	Int.	Δ1	Δ2	J	R(J) A-	Int.	Δ1	Δ2	J	P(J) A+	Int.	Δ1	Δ2	J	P(J) A-	Int.
1			988.48299		1			988.49447		1					1		
2	988.48299	0.9217	1.26785	-987.21514	2	988.49447	0.9252	1.27386	-987.22061	2	982.02518	0.9203	-1.31421		2	982.02518	0.9203
3	989.75084	0.8991	1.25996	-0.00789	3	989.76833	0.9023	1.26712	-0.00674	3	980.71097	0.8523	-1.32138	-0.00717	3	980.71097	0.8523
4	991.01080	0.8723	1.25212	-0.00784	4	991.03545	0.8801	1.26033	-0.00679	4	979.38959	0.8225	-1.33032	-0.00894	4	979.38959	0.8225
5	992.26292	0.8608	1.24370	-0.00842	5	992.29578	0.8572	1.25346	-0.00687	5	978.05926	0.8658	-1.33769	-0.00737	5	978.06300	0.8688
6	993.50663	0.6978	1.23660	-0.00710	6	993.54925	0.8367	1.24682	-0.00664	6	976.72157	0.8738	-1.34537	-0.00768	6	976.72929	0.8749
7	994.74323	0.8279	1.22806	-0.00854	7	994.79607	0.8222	1.23963	-0.00719	7	975.37620	0.8537	-1.35286	-0.00749	7	975.38923	0.8538
8	995.97129	0.8258	1.22028	-0.00778	8	996.03570	0.8119	1.23306	-0.00657	8	974.02334	0.8444	-1.36036	-0.00750	8	974.04287	0.8439
9	997.19157	0.8156	1.21216	-0.00812	9	997.26876	0.7935	1.22606	-0.00700	9	972.66298	0.8285	-1.36782	-0.00746	9	972.68973	0.8232
10	998.40373	0.8000	1.20447	-0.00769	10	998.49482	0.7098	1.21928	-0.00678	10	971.29516	0.8284	-1.37518	-0.00736	10	971.33039	0.7378
11	999.60820	0.7984	1.19618	-0.00829	11	999.71410	0.6938	1.21214	-0.00714	11	969.91998	0.8182	-1.38280	-0.00762	11	969.96507	0.8158
12	1000.80438	0.6775	1.18854	-0.00764	12	1000.92624	0.7944	1.20546	-0.00668	12	968.53718	0.8251	-1.38975	-0.00695	12	968.59326	0.8146
13	1001.99292	0.7788	1.17876	-0.00978	13	1002.13170	0.8091	1.19839	-0.00707	13	967.14743	0.7777	-1.39735	-0.00760	13	967.21515	0.8066
14	1003.17168	0.4805	1.17399	-0.00477	14	1003.33009	0.8161	1.19166	-0.00673	14	965.75008	0.8202	-1.40444	-0.00709	14	965.83124	0.8192
15	1004.34567	0.8064	1.16436	-0.00963	15	1004.52175	0.8073	1.18437	-0.00729	15	964.34563	0.8286	-1.41145	-0.00701	15	964.43998	0.7339
16	1005.51003	0.3675	1.15631	-0.00805	16	1005.70612	0.7229	1.17743	-0.00694	16	962.93418	0.8185	-1.41878	-0.00733	16	963.04393	0.8358
17	1006.66634	0.4039	1.14886	-0.00745	17	1006.88355	0.6886	1.17076	-0.00667	17	961.51540	0.8307	-1.42562	-0.00684	17	961.64146	0.8447
18	1007.81521	0.8237	1.14067	-0.00819	18	1008.05432	0.8056	1.16289	-0.00787	18	960.08978	0.8317	-1.43280	-0.00718	18	960.23293	0.8312
19	1008.95588	0.8420	1.13478	-0.00589	19	1009.21721	0.7283	1.15643	-0.00646	19	958.65698	0.8206	-1.43960	-0.00680	19	958.81834	0.8546
20	1010.09066	0.6855	1.12263	-0.01215	20	1010.37364	0.7026	1.15057	-0.00586	20	957.21738	0.8647	-1.44652	-0.00692	20	957.39784	0.8602
21	1011.21329	0.8666	1.11690	-0.00573	21	1011.52421	0.8437	1.14266	-0.00791	21	955.77086	0.8310	-1.45289	-0.00637	21	955.97165	0.8714
22	1012.33019	0.8761	1.10875	-0.00815	22	1012.66687	0.8698	1.13553	-0.00713	22	954.31797	0.8296	-1.46052	-0.00763	22	954.53944	0.8874
23	1013.43894	0.8635	1.10125	-0.00750	23	1013.80240	0.9002	1.12863	-0.00690	23	952.85745	0.8898	-1.46644	-0.00592	23	953.10151	0.8865
24	1014.54019	0.8905	1.09156	-0.00969	24	1014.93103	0.8911	1.12112	-0.00751	24	951.39101	0.9037	-1.47295	-0.00651	24	951.65803	0.8890
25	1015.63175	0.8900	1.08705	-0.00451	25	1016.05215	0.7913	1.11495	-0.00617	25	949.91805	0.8494	-1.47997	-0.00702	25	950.20865	0.9060
26	1016.71880	0.9234	1.07874	-0.00831	26	1017.16710	0.8084	1.10871	-0.00624	26	948.43808	0.9227	-1.48615	-0.00618	26	948.75382	0.9124
27	1017.79754	0.9303	1.07321	-0.00553	27	1018.27581	0.8585	1.10014	-0.00857	27	946.95193	0.9317	-1.49223	-0.00608	27	947.29336	0.9210
28	1018.87075	0.9663	1.06779	-0.00542	28	1019.37595	0.8414	1.09506	-0.00508	28	945.45970	0.9427	-1.49748	-0.00525	28	945.82760	0.9401
29	1019.93854	0.8755	-1019.93854	-1021.00634	29	1020.47101	0.9330	-1020.47101	-1021.56608	29	943.96222	0.9208	-1.50335	-0.00587	29	944.35600	0.9425
30			0.00000	1019.93854	30			0.00000	1020.47101	30	942.45887	0.8837	-942.45887	-940.95552	30	942.87967	0.9496
31					31					31					31		
32					32					32					32		
33																	

			Q Branch					Q Branch					R-P Diff	R-P Diff	
Δ1	Δ2	J	Q(J) A+ <-- -	Int.	Δ1	Δ2	J	Q(J) A- <-- +	Int.	Δ1	Δ2	J	Xu Calc A+	Obs	Obs-Calc
		1	984.62192		-0.01819		1	984.62806		-0.01051		1	6.49570	-980.71097	-987.20666
-1.31421		2	984.60373		-0.02712	-0.00893	1	984.61756		-0.01618	-0.00567	2	9.09378	9.09341	-0.00037
-1.32138	-0.00717	3	984.57662		-0.03749	-0.01037	1	984.60138		-0.02014	-0.00397	3	11.69167	11.69158	-0.00009
-1.32658	-0.00520	4	984.53913		-0.04657	-0.00908	1	984.58124		-0.02573	-0.00559	4	14.28930	14.28923	-0.00006
-1.33371	-0.00713	5	984.49255		-0.05604	-0.00947	1	984.55550		-0.03081	-0.00508	5	16.88662	16.88672	0.00011
-1.34006	-0.00635	6	984.43651		-0.06521	-0.00917	1	984.52470		-0.03570	-0.00490	6	19.48357	19.48328	-0.00028
-1.34636	-0.00630	7	984.37130		-0.07438	-0.00917	1	984.48899		-0.04116	-0.00546	7	22.08010	22.08025	0.00015
-1.35314	-0.00678	8	984.29693		-0.08374	-0.00936	1	984.44783		-0.04625	-0.00509	8	24.67615	24.67613	-0.00002
-1.35934	-0.00620	9	984.21319		-0.09283	-0.00910	1	984.40159		-0.05100	-0.00476	9	27.27166	27.27159	-0.00007
-1.36532	-0.00598	10	984.12036		-0.10227	-0.00943	1	984.35059		-0.05623	-0.00523	10	29.86657	29.86655	-0.00002
-1.37181	-0.00649	11	984.01809		-0.11107	-0.00881	1	984.29436		-0.06148	-0.00525	11	32.46084	32.46077	-0.00006
-1.37811	-0.00630	12	983.90702		-0.12047	-0.00940	1	984.23288		-0.06598	-0.00450	12	35.05439	35.05431	-0.00008
-1.38391	-0.00580	13	983.78655		-0.12986	-0.00939	1	984.16690		-0.07222	-0.00623	13	37.64718	37.64729	0.00011
-1.39125	-0.00734	14	983.65669		-0.13843	-0.00858	1	984.09468		-0.07621	-0.00399	14	40.23914	40.23750	-0.00164
-1.39605	-0.00480	15	983.51826		-0.14724	-0.00881	1	984.01848		-0.08154	-0.00533	15	42.83022	42.83027	0.00005
-1.40247	-0.00642	16	983.37101		-0.15647	-0.00923	1	983.93694		-0.08668	-0.00514	16	45.42037	45.42025	-0.00011
-1.40853	-0.00606	17	983.21455		-0.16547	-0.00900	1	983.85026		-0.09170	-0.00503	17	48.00951	48.00936	-0.00015
-1.41459	-0.00606	18	983.04907		-0.17418	-0.00871	1	983.75856		-0.09691	-0.00520	18	50.59760	50.59783	
-1.42050	-0.00591	19	982.87489		-0.18273	-0.00855	1	983.66165		-0.10184	-0.00493	19	53.18457	53.18502	
-1.42619	-0.00569	20	982.69215		-0.19150	-0.00876	1	983.55981		-0.10660	-0.00476	20	55.77037	55.77269	
-1.43221	-0.00602	21	982.50066		-0.20163	-0.01014	1	983.45321		-0.11153	-0.00493	21	58.35493	58.35584	
-1.43793	-0.00572	22	982.29902		-0.20929	-0.00766	1	983.34168		-0.11660	-0.00507	22	60.93820	60.93918	
-1.44348	-0.00555	23	982.08973	10R30	-0.21771	-0.00842	1	983.22508		-0.12179	-0.00519	23	63.52013	63.52089	
-1.44937	-0.00589	24	981.87202		-0.22707	-0.00936	1	983.10329		-0.12672	-0.00493	24	66.10064	66.10211	
-1.45483	-0.00546	25	981.64496		-0.23510	-0.00803	1	982.97656		-0.13170	-0.00498	25		68.67982	
-1.46046	-0.00563	26	981.40986		0.32352	0.55862	1	982.84486		-982.84486	-982.71316	26		71.25910	
-1.46576	-0.00530	27	981.73337		-37.77115	-38.09467	1			0.00000	982.84486	27		73.83532	
-1.47160	-0.00584	28	943.96222		-1.50335	36.26780	1			942.87967	942.87967	28		76.41189	
-1.47633	-0.00473	29	942.45887		-942.45887	-940.95552	1	942.87967		-942.87967	-1885.75934	29		1019.93854	
-942.87967	-941.40334	30	0.00000		0.00000	942.45887	1	0.00000		0.00000	942.87967	30		0.00000	
		31	0.00000				1	0.00000				31		0.00000	
		32	0.00000				1	0.00000				32		0.00000	
												33		0.00000	

CD3OH CO-Stretch K=2 E2 n=1 (132)														
	R Branch					P Branch					Q Branch			
J	R(J)	Int.	Δ1	Δ2	J	P(J)	Int.	Δ1	Δ2	J	Q(J)	Int.	Δ1	Δ2
2	989.89541		1.27169		2					2	986.01636	0.9209	-0.02075	
3	991.16709	0.9091	1.26536	-0.00633	3	982.11720	0.9154	-1.32056		3	985.99561	0.9460	-0.02766	-0.00691
4	992.43245	0.8917	1.25832	-0.00704	4	980.79664	0.9070	-1.32743	-0.00687	4	985.96795		-0.03428	-0.00662
5	993.69078	0.8610	1.25110	-0.00722	5	979.46921	0.8583	-1.33382	-0.00639	5	985.93367		-0.04133	-0.00705
6	994.94188	0.8300	1.24378	-0.00732	6	978.13538	0.8790	-1.34065	-0.00683	6	985.89234		-0.04821	-0.00688
7	996.18566	0.8427	1.23736	-0.00642	7	976.79473	0.8672	-1.34717	-0.00652	7	985.84413		-0.05497	-0.00676
8	997.42302	0.8432	1.22991	-0.00745	8	975.44756	0.8577	-1.35376	-0.00659	8	985.78916		-0.06171	-0.00675
9	998.65293	0.7564	1.22336	-0.00655	9	974.09380	0.8161	-1.36030	-0.00654	9	985.72745		-0.06852	-0.00681
10	999.87629	0.8072	1.21612	-0.00724	10	972.73350	ch	-1.36674	-0.00644	10	985.65893		-0.07491	-0.00639
11	1001.09241	0.8176	1.20925	-0.00687	11	971.36676	0.8208	-1.37286	-0.00612	11	985.58402		-0.08192	-0.00701
12	1002.30166	0.8154	1.20234	-0.00691	12	969.99390	0.8159	-1.37945	-0.00659	12	985.50210		-0.08801	-0.00610
13	1003.50400	0.8070	1.19531	-0.00703	13	968.61445	0.8355	-1.38529	-0.00584	13	985.41409		-0.09553	-0.00752
14	1004.69931	0.7918	1.18828	-0.00703	14	967.22916	0.7633	-1.39225	-0.00696	14	985.31856		-0.10063	-0.00510
15	1005.88759	0.8132	1.18164	-0.00664	15	965.83691	0.8432	-1.39692	-0.00467	15	985.21793		-0.10857	-0.00794
16	1007.06924	0.8345	1.17470	-0.00694	16	964.43998	0.7339	-1.40469	-0.00777	16	985.10935		-0.11440	-0.00583
17	1008.24394	0.8450	1.16820	-0.00650	17	963.03529	0.8498	-1.40984	-0.00515	17	984.99495		-0.12070	-0.00630
18	1009.41214	0.8418	1.16010	-0.00810	18	961.62545	0.8619	-1.41556	-0.00572	18	984.87425		-0.12664	-0.00594
19	1010.57224	0.8725	1.15690	-0.00320	19	960.20989	0.8563	-1.42096	-0.00540	19	984.74761		-0.13395	-0.00732
20	1011.72914	0.8170	1.14790	-0.00900	20	958.78693	0.8848	-1.42802	-0.00706	20	984.61366		-0.13773	-0.00378
21	1012.87704	0.8156	1.14348	-0.00442	21	957.36091	0.8797	-1.43126	-0.00324	21	984.47592		-0.14503	-0.00730
22	1014.02052	0.6365	1.13196	-0.01152	22	955.92965	0.8868	-1.43801	-0.00675	22	984.33089		-0.15104	-0.00601
23	1015.15248	0.8990	1.12888	-0.00308	23	954.49164	0.8817	-1.44255	-0.00454	23	984.17986		-0.15749	-0.00646
24	1016.28136	0.8697	1.12216	-0.00672	24	953.04909	0.9212	-1.44796	-0.00541	24	984.02236		-0.16272	-0.00523
25	1017.40352	0.9094	1.11619	-0.00597	25	951.60113	0.9222	-1.45313	-0.00517	25	983.85964		-0.16780	-0.00508
26	1018.51971	0.9198	-1018.51971	-1019.63590	26	950.14799	0.9316	-1.45743	-0.00430	26	983.69184		-983.69184	-983.52404
27			0.00000	1018.51971	27	948.69056	0.9230	-1.46274	-0.00531	27			0.00000	983.69184
28			0.00000	0.00000	28	947.22782	0.9295	-947.22782	-945.76508	28			0.00000	0.00000
29			0.00000	0.00000	29			0.00000	947.22782	29			0.00000	0.00000
30			0.00000	0.00000	30			0.00000	0.00000	30			0.00000	0.00000
31					31					31				
32					32					32				
33														
34														
35														
36														

	R-P Diff	R-P Diff				Calc a-Type
J	Calc	Obs	Obs-Calc	Δ 1	Δ 2	Gd
2	9.09877	9.09877	0.00000		-0.00018	3.89947
3	11.69807	11.69789	-0.00018	-0.00018	0.00033	5.19918
4	14.29710	14.29707	-0.00003	0.00015	0.00011	6.49875
5	16.89582	16.89604	0.00022	0.00026	-0.00032	7.79829
6	19.49415	19.49431	0.00016	-0.00006	-0.00029	9.09761
7	22.09204	22.09186	-0.00019	-0.00035	0.00062	10.39657
8	24.68944	24.68952	0.00008	0.00027	-0.00045	11.69536
9	27.28628	27.28617	-0.00011	-0.00019	0.00019	12.99395
10	29.88250	29.88239	-0.00011	0.00000	0.00002	14.29217
11	32.47805	32.47796	-0.00008	0.00002	-0.00030	15.59012
12	35.07286	35.07251	-0.00036	-0.00027	0.00027	16.88765
13	37.66688	37.66710	0.00022			18.18493
14	40.26005	40.25933	-0.00072			19.48165
15	42.85230	42.85230	0.00000			20.77794
16	45.44358	45.44378	0.00021			22.07406
17	48.03382	48.03404	0.00022			23.36950
18	50.62298	50.62321				24.66436
19	53.21098	53.21133				25.95868
20	55.79776	55.79949				27.25275
21	58.38327	58.38540				28.54628
22	60.96744	60.97143				29.83926
23	63.55022	63.55136				31.13077
24	66.13154	66.13337				32.42124
25		68.71296				33.71165
26		71.29189				35.00128
27		0.00000				18.14703
28		0.00000				
29		0.00000				
30		0.00000				
31		0.00000				
32		0.00000				
33		0.00000				
34		0.00000				
35		0.00000				
36		0.00000				
37						
38						
39						
40						

CD3OH CO-Stretch K=3 E1 n=1 (133)

	R Branch					P Branch					Calc Q	Q Branch			
J	R(J)	Δ1	Δ2	Int.	J	P(J)	Δ1	Δ2	Int.	J	P	Q(J)	Δ1	Δ2	Int.
3	989.10114	1.26274		0.9239	3					3	983.93206	983.93197	-0.02945		0.4949
4	990.36386	1.25501	-0.00773	0.8619	4	978.73335	-1.32930		0.9314	4	983.90239	983.90252	-0.03851	-0.00906	0.7792
5	991.61889	1.24721	-0.00780	0.8367	5	977.40405	-1.33642	-0.00712	0.8864	5	983.86541	983.86401	-0.04417	-0.00566	0.6901
6	992.86610	1.24008	-0.00713	0.7933	6	976.06763	-1.34355	-0.00713	0.8462	6	983.82099	983.81984	-0.05041	-0.00624	0.6482
7	994.10618	1.23201	-0.00807	0.7662	7	974.72408	-1.35072	-0.00717	0.8417	7	983.76920	983.76943	-0.05994	-0.00953	0.8456
8	995.33819	1.22470	-0.00731	0.7744	8	973.37336	-1.35773	-0.00701	0.8130	8	983.71015	983.70949	-0.06558	-0.00564	0.7011
9	996.56289	1.21761	-0.00709	0.7574	9	972.01563	-1.36486	-0.00713	0.7855	9	983.64366	983.64391	-0.07108	-0.00550	0.7998
10	997.78050	1.20878	-0.00883	0.6137	10	970.65077	-1.37201	-0.00715	0.7575	10	983.56996	983.57283	-0.08192	-0.01084	0.7641
11	998.98928	1.20191	-0.00687	0.7229	11	969.27876	-1.37885	-0.00684	0.7607	11	983.48869	983.49091	-0.09022	-0.00830	0.7602
12	1000.19119	1.19417	-0.00774	0.7471	12	967.89991	-1.38580	-0.00695	0.7661	12	983.40034	983.40069	-0.09106	-0.00084	0.9482
13	1001.38536	1.18655	-0.00762	0.7535	13	966.51411	-1.39255	-0.00675	0.7674	13	983.30484	983.30963	-0.10548	-0.01442	0.7535
14	1002.57191	1.17887	-0.00768	0.7449	14	965.12156	-1.39956	-0.00701	0.7792	14	983.20185	983.20415	-0.10493	0.00055	0.8137
15	1003.75078	1.17201	-0.00686	0.7503	15	963.72200	-1.40599	-0.00643	ch	15	983.09188	983.09922	-0.12473	-0.01980	0.8186
16	1004.92279	1.16312	-0.00889	0.7015	16	962.31601	-1.41264	-0.00665	0.7832	16	982.97500	982.97449	-0.12410	0.00063	0.8481
17	1006.08591	1.15607	-0.00705	0.7610	17	960.90337	-1.41953	-0.00689	0.7663	17	982.85063	982.85039	-0.12161	0.00249	0.8879
18	1007.24198	1.14857	-0.00750	0.7463	18	959.48384	-1.42595	-0.00642	0.8000	18	982.71918	982.72878	-0.12400	-0.00239	0.9391
19	1008.39055	1.14087	-0.00770	0.7891	19	958.05789	-1.43288	-0.00693	0.7963	19	982.58029	982.60478	-0.16712	-0.04312	0.9229
20	1009.53142	1.13323	-0.00764	0.8023	20	956.62501	-1.43841	-0.00553	0.7283	20	982.43512	982.43766	-0.14141	0.02571	0.8580
21	1010.66465	1.12579	-0.00744	0.8256	21	955.18660	-1.44511	-0.00670	0.8308	21	982.28275	982.29625	-0.13960	0.00181	0.8968
22	1011.79044	1.11811	-0.00768	0.8412	22	953.74149	-1.45173	-0.00662	0.8348	22	982.12305	982.15665	-0.19307	-0.05347	0.8299
23	1012.90855	1.11197	-0.00614	0.8495	23	952.28976	-1.45737	-0.00564	0.8228	23	981.95692	981.96358	-0.16196	0.03111	0.9297
24	1014.02052	1.10173	-0.01024	0.6365	24	950.83239	-1.46366	-0.00629	0.8088	24	981.78425	981.80162	-0.19555	-0.03359	0.9154
25	1015.12225	1.09597	-0.00576	0.8829	25	949.36873	-1.47024	-0.00658	0.7541	25	981.60403	981.60607	-0.18548	0.01007	0.8212
26	1016.21822	1.08752	-0.00845	0.7995	26	947.89849	-1.47607	-0.00583	0.8926	26	981.41685	981.42059	-0.19204	-0.00656	0.8531
27	1017.30574	1.08066	-0.00686	0.8990	27	946.42242	-1.48181	-0.00574	0.9028	27	981.22332	981.22855	-0.17587	0.01617	0.8128
28	1018.38640	1.07295	-0.00771	0.8016	28	944.94061	-1.48780	-0.00599	0.9165	28	981.02289	981.05268	-0.17186	0.00401	0.9495
29	1019.45935	1.06518	-0.00777	0.8986	29	943.45281	-1.49352	-0.00572	0.9308	29	980.81600	980.88082	-0.20783	-0.03577	0.8767
30	1020.52453	1.05803	-0.00715	0.9185	30	941.95929	-1.49935	-0.00583	0.9304	30	980.60222	980.67319	-0.26937	-0.06174	0.8949
31	1021.58256	1.05278	-0.00525	0.9463	31	940.45994	-1.50480	-0.00545	0.9421	31		980.40382	-0.23547	0.03390	0.8728
32	1022.63534	1.04699	-0.00579	0.8087	32	938.95514	-1.51096	-0.00616	0.9211	32		980.16835	-0.24271	-0.00724	0.8944
33	1023.68233	-1023.68233	-1024.72932	0.9525	33	937.44418	-937.44418	-935.93322	0.9612	33		979.92564	-0.24143	0.00128	0.9211
34										34		979.68421	-0.24372	-0.00229	0.9325
35										35		979.44049	-0.20306	0.04066	0.8281
36										36		979.23743	-0.27563	-0.07257	0.9225
										37		978.96180	-0.26164	0.01399	0.7702
										38		978.70016	-0.27537	-0.01373	0.7798
										39		978.42479	-0.10679	0.16858	0.8148
										40		978.31800	-978.31800	-978.21121	0.9264

	R-P Diff	R-P Diff	R-P Diff				Calc a-Type
J	Xu Calc	Calc	Obs	Obs-Calc	Δ 1	Δ 2	Gd
3	11.69733	11.69740	11.69709	-0.00031			5.19871
4	14.296173	14.29625	14.29625	0.00000	0.00031	-0.00026	6.49834
5	16.894676	16.89476	16.89481	0.00005	0.00005	-0.00023	7.79778
6	19.492782	19.49287	19.49274	-0.00013	-0.00018	0.00035	9.09691
7	22.090423	22.09051	22.09055	0.00004	0.00017	-0.00042	10.39584
8	24.687541	24.68763	24.68742	-0.00021	-0.00025	0.00043	11.69452
9	27.284073	27.28416	27.28413	-0.00003	0.00018	0.00040	12.99291
10	29.879957	29.88004	29.88059	0.00055	0.00058	-0.00116	14.29120
11	32.475132	32.47520	32.47517	-0.00003	-0.00058	0.00065	15.58898
12	35.069534	35.06959	35.06963	0.00004	0.00007	0.00011	16.88623
13	37.663102	37.66314	37.66336	0.00022	0.00018	-0.00029	18.18328
14	40.255773	40.25579	40.25590	0.00011	-0.00011	42.84741	19.47985
15	42.847485		42.84741	42.84741	42.84730	-42.84730	20.77587
16	45.438176		45.43895	45.43895			22.07163
17	48.027782		48.02802	48.02802			23.36679
18	50.616241		50.61697	50.61697			24.66129
19	53.203491		53.20395	53.20395			25.95528
20	55.789469		55.78993	55.78993			27.24852
21	58.374112		58.37489				28.54126
22	60.957358		60.95805				29.83329
23	63.539145		63.53982				31.12453
24	66.119409		66.12203				32.41552
25			68.69983				33.70554
26			71.27761				34.99443
27			73.85293				36.28271
28			76.42711				37.57008
29			78.99941				38.85671
30			81.56939				40.14228
31			84.13838				
32			1022.63534				
33			1023.68233				
			0.00000				
			0.00000				
			0.00000				
			0.00000				
			0.00000				
			0.00000				

CD3OH CO-Stretch K=4 A n=1 (134)															
	R Branch					P Branch					Calc Q	Q Branch			
J	R(J)	Δ1	Δ2	Int.	J	P(J)	Δ1	Δ2	Int.	J	P	Q(J)		Δ2	Int.
4	990.13387	1.25434		0.9188	4					4	983.67226	983.67299	-0.03692		0.5592
5	991.38821	1.24669	-0.00765	0.8562	5	977.17469	-1.33547		0.6929	5	983.63615	983.63607	-0.04487	-0.00795	0.7020
6	992.63490	1.23898	-0.00771	0.8184	6	975.83922	-1.34404	-0.00857	0.8712	6	983.59115	983.59120	-0.05269	-0.00782	0.7344
7	993.87388	1.23142	-0.00756	0.7729	7	974.49518	-1.35106	-0.00702	0.8237	7	983.53885	983.53851	-0.05985	-0.00716	0.7702
8	995.10530	1.22384	-0.00758	0.7384	8	973.14412	-1.35830	-0.00724	0.7708	8	983.47904	983.47866	-0.06682	-0.00697	0.7073
9	996.32914	1.21540	-0.00844	0.6260	9	971.78582	-1.36523	-0.00693	0.7304	9	983.41204	983.41184	-0.07726	-0.01044	0.7216
10	997.54454	1.20849	-0.00691	0.4924	10	970.42059	-1.37242	-0.00719	0.7310	10	983.33741	983.33458	-0.07942	-0.00216	0.7817
11	998.75303	1.20043	-0.00806	0.7084	11	969.04817	-1.37946	-0.00704	0.7399	11	983.25537	983.25516	-0.08879	-0.00937	7448/10R
12	999.95346	1.19279	-0.00764	0.6783	12	967.66871	-1.38637	-0.00691	0.7413	12	983.16619	983.16637	-0.09708	-0.00829	0.8412
13	1001.14625	1.18516	-0.00763	0.6351	13	966.28234	-1.39347	-0.00710	0.7302	13	983.06937	983.06929	-0.10387	-0.00679	0.8518
14	1002.33141	1.17737	-0.00779	0.6944	14	964.88887	-1.39985	-0.00638	0.4967	14	982.96568	982.96542	-0.10815	-0.00428	0.8086
15	1003.50878	1.16956	-0.00781	0.6987	15	963.48902	-1.40687	-0.00702	0.7349	15	982.85453	982.85727	-0.11775	-0.00960	0.8829
16	1004.67834	1.16185	-0.00771	0.7185	16	962.08215	-1.41347	-0.00660	0.7257	16	982.73623	982.73952	-0.12856	-0.01081	0.9281
17	1005.84019	1.15428	-0.00757	0.7151	17	960.66868	-1.42024	-0.00677	0.7406	17	982.61057	982.61096	-0.13629	-0.00773	0.8927
18	1006.99447	1.14651	-0.00777	0.7364	18	959.24844	-1.42665	-0.00641	0.7612	18	982.47780	982.47467	-0.13558	0.00071	0.8909
19	1008.14098	1.13857	-0.00794	0.7401	19	957.82179	-1.43272	-0.00607	0.7576	19	982.33873	982.33909	-982.33909	-982.20351	0.8651
20	1009.27955	1.13126	-0.00731	0.7670	20	956.38907	-1.44113	-0.00841	0.6668	20	982.19039		0.00000	982.33909	
21	1010.41081	1.12338	-0.00788	0.7875	21	954.94794	-1.44490	-0.00377	0.7428	21	982.03738		0.00000	0.00000	
22	1011.53419	1.11676	-0.00662	0.8093	22	953.50304	-1.45287	-0.00797	0.8036	22	981.87597		0.00000	0.00000	
23	1012.65095	1.10696	-0.00980	0.5458	23	952.05017	-1.45830	-0.00543	0.7946	23	981.70839		0.00000	0.00000	
24	1013.75791	1.10029	-0.00667	0.8377	24	950.59187	-1.46443	-0.00613	0.8245	24	981.53373		0.00000	0.00000	
25	1014.85820	1.09289	-0.00740	0.8190	25	949.12744	-1.47087	-0.00644	0.8396	25	981.35158		0.00000	0.00000	
26	1015.95109	1.08541	-0.00748	0.8669	26	947.65657	-1.47678	-0.00591	0.8719	26	981.16294		0.00000	0.00000	
27	1017.03650	1.07754	-0.00787	.6870G*B	27	946.17979	-1.48259	-0.00581	0.8837	27	980.96773		0.00000	0.00000	
28	1018.11404	1.07007	-0.00747	0.8867	28	944.69720	-1.48862	-0.00603	0.9016	28	980.76557		0.00000	0.00000	
29	1019.18411	1.06253	-0.00754	0.8514	29	943.20858	-1.49428	-0.00566	0.9170	29	980.55672		0.00000	0.00000	
30	1020.24664	1.05416	-0.00837	0.9095	30	941.71430	-1.49981	-0.00553	0.9204	30	1211.29360		0.00000	0.00000	
31	1021.30080	1.04811	-0.00605	0.7940	31	940.21449	-940.21449	-938.71468	0.9247	31	510.50738		0.00000	0.00000	
32	1022.34891	-1022.34891	-1023.39702	0.8983	32					32			0.00000	0.00000	
33		0.00000	1022.34891							33			0.00000	0.00000	
34		0.00000	0.00000							34			0.00000	0.00000	
35		0.00000	0.00000							35			0.00000	0.00000	
36		0.00000	0.00000							36			0.00000	0.00000	
		0.00000	0.00000							37			0.00000	0.00000	
										38			0.00000	0.00000	
										39			0.00000	0.00000	
										40			0.00000	0.00000	

	R-P Diff	R-P Diff				Calc a-Type
J	Calc	Obs	Obs-Calc	Δ1	Δ2	Gd
4	14.29517	14.29465	-0.00052			6.49757
5	16.89341	16.89303	-0.00038	0.00014	-0.00020	7.79693
6	19.49122	19.49078	-0.00044	-0.00006	0.00004	9.09597
7	22.08852	22.08806	-0.00046	-0.00002	-0.00005	10.39473
8	24.68524	24.68471	-0.00053	-0.00007	0.00024	11.69322
9	27.28133	27.28097	-0.00036	0.00017	-0.00069	12.99145
10	29.87671	29.87583	-0.00088	-0.00052	0.00078	14.28924
11	32.47131	32.47069	-0.00062	0.00026	-0.00012	15.58666
12	35.06507	35.06459	-0.00048	0.00014	-0.00035	16.88385
13	37.65792	37.65723	-0.00069	-0.00021	0.00037	18.18050
14	40.24979	40.24926	-0.00053	0.00016	-0.00014	19.47666
15	42.84061	42.84010	-0.00051	0.00002	45.43039	20.77238
16		45.42990	45.42990	45.43041	-45.43041	22.06755
17		48.01840	48.01840			23.36213
18		50.60540	50.60540			24.65601
19		53.19304	53.19304			25.94966
20		55.77651	55.77651			27.24245
21		58.36064	58.36064			28.53434
22		60.94232				29.82580
23		63.52351				31.11652
24		66.10134				32.40629
25		68.67841				33.69501
26		71.25389				34.98315
27		73.82792				36.27053
28		76.39974				37.55699
29		78.96962				38.84242
30		1020.24664				271.07911
31		1021.30080				510.50738
32		1022.34891				
33		0.00000				
34		0.00000				
35		0.00000				
36		0.00000				
37		0.00000				
38		0.00000				
39		0.00000				
40		0.00000				

CD3OH CO-Stretch K=3 E2 n=1 (123)														
	R Branch					P Branch					Q Branch			
J	R(J)	Int.	Δ1	Δ2	J	P(J)	Int.	Δ1	Δ2	J	Q(J)	Int.	Δ1	Δ2
3	990.20931	0.8077	1.26169		3					3	985.03884		-0.02937	
4	991.47100	0.7956G*	1.25442	-0.00726	4	979.83946	0.8220	-1.32876		4	985.00947		-0.03676	-0.00739
5	992.72542	0.8420	1.24680	-0.00762	5	978.51069	0.7569	-1.33600	-0.00724	5	984.97271		-0.04555	-0.00879
6	993.97223	0.8233	1.23904	-0.00776	6	977.17469	0.6929	-1.34505	-0.00905	6	984.92717		-0.05253	-0.00699
7	995.21127	0.7998	1.23143	-0.00761	7	975.82964	0.8203	-1.35167	-0.00662	7	984.87463		-0.06012	-0.00758
8	996.44270	0.7857	1.22373	-0.00770	8	974.47797	0.8103	-1.35903	-0.00736	8	984.81452		-0.06749	-0.00738
9	997.66643	0.7590	1.21611	-0.00762	9	973.11894	0.7934	-1.36614	-0.00711	9	984.74702		-0.07491	-0.00741
10	998.88254	0.7199	1.20841	-0.00770	10	971.75280	0.7883	-1.37328	-0.00714	10	984.67212		-0.08228	-0.00737
11	1000.09095	0.7603	1.20109	-0.00732	11	970.37952	0.7841	-1.38037	-0.00709	11	984.58984		-0.08965	-0.00737
12	1001.29204	0.6221	1.19261	-0.00848	12	968.99915	0.7815	-1.38748	-0.00711	12	984.50020		-0.09697	-0.00732
13	1002.48465	0.7534	1.18537	-0.00724	13	967.61167	0.7735	-1.39435	-0.00687	13	984.40323		-0.10449	-0.00752
14	1003.67002	0.6870	1.17778	-0.00759	14	966.21732	0.7586	-1.40145	-0.00710	14	984.29874		-0.11180	-0.00731
15	1004.84780	0.7388	1.16995	-0.00783	15	964.81586	0.7638	-1.40843	-0.00698	15	984.18694		-0.11876	-0.00696
16	1006.01775	0.7664	1.16232	-0.00763	16	963.40743	0.7933	-1.41492	-0.00649	16	984.06818		-0.12626	-0.00750
17	1007.18008	0.7688	1.15490	-0.00742	17	961.99251	0.7708	-1.42199	-0.00707	17	983.94192		-0.13333	-0.00707
18	1008.33498	0.7956	1.14706	-0.00784	18	960.57052	0.7917	-1.42864	-0.00665	18	983.80858		-0.14059	-0.00725
19	1009.48204	0.8066	1.13945	-0.00761	19	959.14188	0.8019	-1.43536	-0.00672	19	983.66800		-0.14762	-0.00703
20	1010.62149	0.8077	1.13191	-0.00754	20	957.70652	0.8200	-1.44175	-0.00639	20	983.52038		-0.15463	-0.00701
21	1011.75340	0.8251	1.12364	-0.00827	21	956.26477	0.8329	-1.44825	-0.00650	21	983.36575		-0.16198	-0.00735
22	1012.87704	0.8156	1.11746	-0.00618	22	954.81652	0.8335	-1.45487	-0.00662	22	983.20377		-0.16873	-0.00675
23	1013.99450	0.8305	1.10935	-0.00811	23	953.36165	0.8480	-1.46113	-0.00626	23	983.03505		-0.17533	-0.00660
24	1015.10385	0.8698	1.10179	-0.00756	24	951.90052	0.8738	-1.46741	-0.00628	24	982.85972		-0.18300	-0.00767
25	1016.20564	0.8383	1.09578	-0.00601	25	950.43310	0.7876	-1.47410	-0.00669	25	982.67672		-0.18852	-0.00552
26	1017.30142	0.7479	1.08498	-0.01080	26	948.95900		-1.47916	-0.00505	26	982.48820		-0.19622	-0.00770
27	1018.38640	0.8018	1.08057	-0.00441	27	947.47984	0.9116	-1.48585	-0.00669	27	982.29198		-982.29198	-982.09576
28	1019.46697	0.9127	1.07298	-0.00759	28	945.99399	0.9117	-1.49184	-0.00599	28			0.00000	982.29198
29	1020.53995	0.9341	1.06595	-0.00703	29	944.50215	0.9256	-1.49677	-0.00493	29			0.00000	0.00000
30	1021.60591	0.8601	1.05774	-0.00821	30	943.00538	0.9441	-1.50255	-0.00578	30			0.00000	0.00000
31	1022.66365	0.9051	-1022.66365	-1023.72139	31	941.50283	0.9448	-1.50615	-0.00360	31				
32			0.00000	1022.66365	32	939.99668	0.9288	-939.99668	-938.49053	32				
33			0.00000	0.00000				0.00000	939.99668					
34			0.00000	0.00000				0.00000	0.00000					
35								0.00000	0.00000					
36								0.00000	0.00000					

	R-P Diff	R-P Diff					Calc a-Type
J	Calc	Obs	Obs-Calc	Δ1	Δ2	J	Gd
3	11.69805	11.69862	0.00057	-0.00138		3	5.19939
4	14.29712	14.29631	-0.00081	0.00070	0.00209	4	6.49878
5	16.89589	16.89578	-0.00011	0.00005	-0.00065	5	7.79802
6	19.49431	19.49425	-0.00005	0.00006	0.00001	6	9.09752
7	22.09232	22.09233	0.00000	0.00002	-0.00004	7	10.39666
8	24.68987	24.68990	0.00002	-0.00002	-0.00004	8	11.69558
9	27.28691	27.28691	0.00000	0.00002	0.00004	9	12.99422
10	29.88337	29.88339	0.00002	0.00005	0.00004	10	14.29260
11	32.47921	32.47928	0.00007	0.00028	0.00023	11	15.59070
12	35.07437	35.07473	0.00036	-0.00036	-0.00065	12	16.88853
13	37.66879	37.66879	0.00000	0.00017	0.00053	13	18.18591
14	40.26242	40.26259	0.00017	-0.00008	-0.00025	14	19.48288
15	42.85520	42.85529	0.00009	0.00006	0.00014	15	20.77951
16	45.44708	45.44723	0.00015	0.00004	-0.00002	16	22.07567
17	48.03800	48.03819	0.00019	0.00036	0.00031	17	23.37140
18	50.62791	50.62846	0.00055	-0.00002	-0.00038	18	24.66670
19	53.21674	53.21727	0.00052	0.00000	0.00002	19	25.96148
20	55.80445	55.80497	0.00052	0.00026	0.00026	20	27.25561
21	58.39097	58.39175	0.00078	-0.00051	-0.00077	21	28.54923
22	60.97625	60.97652	0.00027	0.00089	0.00140	22	29.84212
23	63.56023	63.56140	0.00116	-0.00116	-0.00206	23	31.13453
24	66.14285	66.14485			0.00116	24	32.42662
25		68.72580				25	33.71772
26		71.30743				26	35.00836
27		73.88425				27	36.29799
28		76.46160				28	37.58653
29		79.03713				29	38.87475
30		81.60923				30	40.16167
31		1022.66365				31	
32		0.00000				32	
33		0.00000				33	
34		0.00000				34	
35		0.00000				35	
36		0.00000				36	
37						37	
38						38	
39						39	
40						40	

C.2 MOSAA assigned series outputs for the spectrum of CD_3OH in the 910-1300 cm^{-1} region.

There are 11 series assigned in this testing. The format of the outputs from MOSAA is similar to the one used in the spreadsheet files. Output of each series (if it has a Q branch) is split into two pages manually just for reading purposes.

The basic format used in the outputs here are almost the same as the outputs of spectrum of $CH_3^{18}OH$ in the 900-1100 cm^{-1} region. One more column section is added[1] to show the difference between the calculated R-P combination difference and the observed R-P combination difference for each J.

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[1] Only done for the n=1 region

K=0 n=0 A+ (010)A

R_branch

J	wv	delta1	delta2	intens	Comm
0.	987.123420	1.289310		0.919400	
1.	988.412730	1.282560	-0.006750	0.869700	
2.	989.695290	1.275550	-0.007010	0.812000	
3.	990.970840	1.268500	-0.007050	0.758500	
4.	992.239340	1.261240	-0.007260	0.744400	
5.	993.500580	1.253670	-0.007570	0.649300	
6.	994.754250	1.246170	-0.007500	0.671200	
7.	996.000420	1.238360	-0.007810	0.635500	
8.	997.238780	1.230430	-0.007930	0.614800	
9.	998.469210	1.222220	-0.008210	0.588700	
10.	999.691430	1.213980	-0.008240	0.608300	
11.	1000.905410	1.205260	-0.008720	0.578100	
12.	1002.110670	1.196780	-0.008480	0.592800	
13.	1003.307450	1.187810	-0.008970	0.593000	
14.	1004.495260	1.178260	-0.009550	0.561800	
15.	1005.673520	1.169490	-0.008770	0.584700	
16.	1006.843010	1.159900	-0.009590	0.610900	
17.	1008.002910	1.149620	-0.010280	0.581700	
18.	1009.152530	1.139400	-0.010220	0.653200	
19.	1010.291930	1.128130	-0.011270	0.543800	
20.	1011.420060	1.115400	-0.012730	0.650800	
21.	1012.535460	1.116070	0.000670	0.493900	
22.	1013.651530			0.538700	

P_branch

J	wv	delta1	delta2	intens	Comm
1.	984.521900	-1.308500		0.818800	
2.	983.213400	-1.315820	-0.007320	0.727300	
3.	981.897580	-1.322950	-0.007130	0.802100	
4.	980.574630	-1.329640	-0.006690	0.774600	
5.	979.244990	-1.335910	-0.006270	0.713500	
6.	977.909080	-1.342490	-0.006580	0.657900	
7.	976.566590	-1.348960	-0.006470	0.684300	
8.	975.217630	-1.355550	-0.006590	0.661400	
9.	973.862080	-1.362120	-0.006570	0.646700	
10.	972.499960	-1.368750	-0.006630	0.638600	
11.	971.131210	-1.375410	-0.006660	0.627800	
12.	969.755800	-1.382120	-0.006710	0.610200	
13.	968.373680	-1.388980	-0.006860	0.614600	
14.	966.984700	-1.395860	-0.006880	0.637100	
15.	965.588840	-1.402870	-0.007010	0.640200	
16.	964.185970	-1.409910	-0.007040	0.638200	
17.	962.776060	-1.417130	-0.007220	0.657700	
18.	961.358930	-1.424210	-0.007080	0.676000	
19.	959.934720	-1.431970	-0.007760	0.631000	
20.	958.502750	-1.439130	-0.007160	0.705300	
21.	957.063620	-1.446700	-0.007570	0.578900	
22.	955.616920	-1.454540	-0.007840	0.711600	
23.	954.162380	-1.462450	-0.007910	0.664200	
24.	952.699930	-1.469870	-0.007420	0.744500	
25.	951.230060	-1.477760	-0.007890	0.802000	
26.	949.752300	-1.485960	-0.008200	0.816900	
27.	948.266340	-1.493130	-0.007170	0.839700	
28.	946.773210	-1.500820	-0.007690	0.816500	
29.	945.272390	-1.508760	-0.007940	0.831400	
30.	943.763630	-1.516900	-0.008140	0.657400	
31.	942.246730	-1.524690	-0.007790	0.877800	
32.	940.722040			0.916000	

```
K=0    n=0     E1                                                   (030)E

 R_branch                                                    |  P_branch
 J         wv        delta1       delta2      intens   Comm  |    J        wv         delta1       delta2      intens   Comm
 0.     986.820000  1.271500                  0.906700       |
 1.     988.091500  1.260080   -0.011420     0.859800       |    1.    984.224320  -1.312520                 0.748100
 2.     989.351580  1.255090   -0.004990     0.828100       |    2.    982.911800  -1.319440   -0.006920     0.799800
 3.     990.606670  1.250620   -0.004470     0.755400       |    3.    981.592360  -1.323800   -0.004360     0.772100
 4.     991.857290  1.244810   -0.005810     0.680600       |    4.    980.268560  -1.329370   -0.005570     0.642100
 5.     993.102100  1.237820   -0.006990     0.626100       |    5.    978.939190  -1.334970   -0.005600     0.659300
 6.     994.339920  1.230130   -0.007690     0.554400       |    6.    977.604220  -1.341720   -0.006750     0.618100
 7.     995.570050  1.221890   -0.008240     0.548800       |    7.    976.262500  -1.348730   -0.007010     0.585300
 8.     996.791940  1.213480   -0.008410     0.518600       |    8.    974.913770  -1.355830   -0.007100     0.554100
 9.     998.005420  1.204850   -0.008630     0.504800       |    9.    973.557940  -1.363230   -0.007400     0.535600
10.     999.210270  1.195970   -0.008880     0.494200       |   10.    972.194710  -1.370570   -0.007340     0.535900
11.    1000.406240  1.187000   -0.008970     0.479500       |   11.    970.824140  -1.380130   -0.009560     0.523300
12.    1001.593240  1.178130   -0.008870     0.436600       |   12.    969.444010  -1.383520   -0.003390     0.261000
13.    1002.771370  1.169030   -0.009100     0.495800       |   13.    968.060490  -1.393290   -0.009770     0.503100
14.    1003.940400  1.159920   -0.009110     0.496900       |   14.    966.667200  -1.400790   -0.007500     0.519200
15.    1005.100320  1.150700   -0.009220     0.505100       |   15.    965.266410  -1.408690   -0.007900     0.538100
16.    1006.251020  1.141750   -0.008950     0.468800       |   16.    963.857720  -1.415990   -0.007300     0.317000
17.    1007.392770  1.132760   -0.008990     0.519900       |   17.    962.441730  -1.423810   -0.007820     0.535900
18.    1008.525530  1.123610   -0.009150     0.563400       |   18.    961.017920  -1.431470   -0.007660     0.579200
19.    1009.649140  1.114740   -0.008870     0.582400       |   19.    959.586450  -1.439060   -0.007590     0.597400
20.    1010.763880  1.106010   -0.008730     0.583100       |   20.    958.147390  -1.446820   -0.007760     0.512300
21.    1011.869890  1.097840   -0.008170     0.627200       |   21.    956.700570  -1.454340   -0.007520     0.641800
22.    1012.967730  1.088670   -0.009170     0.549000       |   22.    955.246230  -1.461520   -0.007180     0.661300
23.    1014.056400  1.083440   -0.005230     0.638600       |   23.    953.784710  -1.471110   -0.009590     0.655800
24.    1015.139840  1.078380   -0.005060     0.714300       |   24.    952.313600  -1.481210   -0.010100     0.718700
25.    1016.218220  1.065310   -0.013070     0.799500       |   25.    950.832390  -1.486880   -0.005670     0.808800
26.    1017.283530  1.053440   -0.011870     0.925200       |   26.    949.345510  -1.493470   -0.006590     0.920300
27.    1018.336970  1.043710   -0.009730     0.881400       |   27.    947.852040  -1.500880   -0.007410     0.915300
28.    1019.380680  1.035960   -0.007750     0.895600       |   28.    946.351160                             0.914800
29.    1020.416640  1.034710   -0.001250     0.953100       |
30.    1021.451350                            0.819000       |
```

K=1 n=1 E1 (121)E1

R_branch

J	wv	delta1	delta2	intens	Comm
1.	987.761300	1.278350		0.924900	
2.	989.039650	1.270780	-0.007570	0.892400	
3.	990.310430	1.263610	-0.007170	0.869800	
4.	991.574040	1.256070	-0.007540	0.841100	
5.	992.830110	1.248840	-0.007230	0.814600	
6.	994.078950	1.241360	-0.007480	0.799900	
7.	995.320310	1.234060	-0.007300	0.761900	c
8.	996.554370	1.226130	-0.007930	0.759500	c
9.	997.780500	1.219710	-0.006420	0.613700	c
10.	999.000210	1.211940	-0.007770	0.746600	
11.	1000.212150	1.204490	-0.007450	0.739800	
12.	1001.416640	1.197450	-0.007040	0.732600	c
13.	1002.614090	1.189350	-0.008100	0.681400	c
14.	1003.803440	1.182330	-0.007020	0.731500	
15.	1004.985770	1.174990	-0.007340	0.743300	
16.	1006.160760	1.167630	-0.007360	0.746300	c
17.	1007.328390	1.160250	-0.007380	0.738200	
18.	1008.488640	1.153000	-0.007250	0.773700	
19.	1009.641640	1.145670	-0.007330	0.788400	
20.	1010.787310	1.138350	-0.007320	0.807600	
21.	1011.925660	1.132440	-0.005910	0.781200	
22.	1013.058100	1.126570	-0.005870	0.812000	
23.	1014.184670	1.112580	-0.013990	0.836800	
24.	1015.297250	1.102950	-0.009630	0.740200	
25.	1016.400200	1.096710	-0.006240	0.954600	
26.	1017.496910	1.089590	-0.007120	0.938900	
27.	1018.586500			0.831600	

P_branch

J	wv	delta1	delta2	intens	Comm
3.	981.261920	-1.321610		0.896800	
4.	979.940310	-1.328570	-0.006960	0.823200	
5.	978.611740	-1.335850	-0.007280	0.843600	
6.	977.275890	-1.342870	-0.007020	0.819700	
7.	975.933020	-1.349620	-0.006750	0.797500	
8.	974.583400	-1.356870	-0.007250	0.791600	c
9.	973.226530	-1.363570	-0.006700	0.786100	c
10.	971.862960	-1.371160	-0.007590	0.745900	c
11.	970.491800	-1.376790	-0.005630	0.591300	
12.	969.115010	-1.384140	-0.007350	0.727100	
13.	967.730870	-1.390700	-0.006560	0.729200	c
14.	966.340170	-1.397350	-0.006650	0.763900	c
15.	964.942820	-1.404180	-0.006830	0.766400	
16.	963.538640	-1.410320	-0.006140	0.735500	
17.	962.128320	-1.417040	-0.006720	0.780700	c
18.	960.711280	-1.423990	-0.006950	0.792200	
19.	959.287290			0.738500	

(121)E1

	RP_cal	RP_obs	diff	J	wv	delta1	delta2	intens	Comm
					Q_branch				
1.	6.499670	6.499380	0.000290						
2.	9.099345	9.099340	0.000005						
3.	11.698826	11.698690	0.000136						
4.	14.298059	14.298150	-0.000091						
5.	16.896988	16.897090	-0.000102						
6.	19.495557	19.495550	0.000007						
7.	22.093713	22.093780	-0.000067	7.	984.982370	-0.059890		0.437400	c
8.	24.691397	24.691410	-0.000013	8.	984.922480	-0.064280	-0.004390	0.488200	c
9.	27.288554	27.288700	-0.000146	9.	984.858200	-0.073620	-0.009340	0.761000	c
10.	29.885130	29.885200	-0.000070	10.	984.784580	-0.080820	-0.007200	0.350500	
11.	32.481068	32.481280	-0.000212	11.	984.703760	-0.084690	-0.003870	0.637900	
12.	35.076311	35.076470	-0.000159	12.	984.619070	-0.090370	-0.005680	0.796200	c
13.	37.670803	37.671270	-0.000467	13.	984.528700	-0.101440	-0.011070	0.892500	c
14.	40.264488	40.264800	-0.000312	14.	984.427260	-0.105110	-0.003670	0.807700	
15.	42.857310	42.857450	-0.000140	15.	984.322150	-0.116770	-0.011660	0.789300	
16.	45.449209	45.449480	-0.000271	16.	984.205380	-0.121740	-0.004970	0.873000	c
17.	48.040130	48.041100	-0.000970	17.	984.083640			0.807000	
18.									
19.									
20.									
21.									
22.									
23.									
24.									
25.									
26.									
27.									

K=4   n=1   E1   (124)E1

R_branch

J	wv	delta1	delta2	intens	Comm
4.	991.433860	1.254290		0.938200	
5.	992.688150	1.246690	-0.007600	0.740400	c
6.	993.934840	1.238920	-0.007770	0.722400	c
7.	995.173760	1.231340	-0.007580	0.813900	c
8.	996.405100	1.223730	-0.007610	0.809300	
9.	997.628830	1.216020	-0.007710	0.794500	c
10.	998.844850	1.208340	-0.007680	0.762700	
11.	1000.053190	1.200680	-0.007660	0.756800	
12.	1001.253870	1.192970	-0.007710	0.774500	c
13.	1002.446840	1.185500	-0.007470	0.775400	
14.	1003.632340	1.177780	-0.007720	0.762400	
15.	1004.810120	1.170360	-0.007420	0.755300	c
16.	1005.980480	1.163530	-0.006830	0.759800	c
17.	1007.144010	1.154940	-0.008590	0.722400	
18.	1008.298950	1.148870	-0.006070	0.776900	
19.	1009.447820	1.142670	-0.006200	0.798500	
20.	1010.590490	1.138650	-0.004020	0.649500	c
21.	1011.729140	1.137640	-0.001010	0.817000	c
22.	1012.866780	1.127720	-0.009920	0.885900	
23.	1013.994500	1.114460	-0.013260	0.830500	
24.	1015.108960			0.942500	

P_branch

J	wv	delta1	delta2	intens	Comm
5.	978.474640	-1.337460		0.927200	
6.	977.137180	-1.343850	-0.006390	0.856800	c
7.	975.793330	-1.351550	-0.007700	0.863200	c
8.	974.441780	-1.358910	-0.007360	0.839100	c
9.	973.082870	-1.366090	-0.007180	0.801400	
10.	971.716780	-1.373250	-0.007160	0.801900	c
11.	970.343530	-1.380180	-0.006930	0.799600	
12.	968.963350	-1.386880	-0.006700	0.792000	
13.	967.576470	-1.394630	-0.007750	0.704800	c
14.	966.181840	-1.401500	-0.006870	0.706200	
15.	964.780340	-1.408030	-0.006530	0.770900	
16.	963.372310	-1.414820	-0.006790	0.798300	c
17.	961.957490	-1.421470	-0.006650	0.797800	c
18.	960.536020	-1.427960	-0.006490	0.807900	
19.	959.108060	-1.434550	-0.006590	0.716600	
20.	957.673510	-1.439920	-0.005370	0.815000	
21.	956.233590	-1.444810	-0.004890	0.833700	c
22.	954.788780	-1.447590	-0.002780	0.843800	c
23.	953.341190			0.813300	

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                                          (124)E1

|                                                                  Q_branch

|          RP_cal         RP_obs          diff        | J       wv          delta1      delta2      intens   Comm
|  4.     14.296166      14.296680      -0.000514     | 4.   984.976210  -0.040210                0.731900
|  5.     16.894768      16.894820      -0.000052     | 5.   984.936000  -0.046270   -0.006060    0.582900    c
|  6.     19.493021      19.493060      -0.000039     | 6.   984.889730  -0.052130   -0.005860    0.506900    c
|  7.     22.090870      22.090890      -0.000020     | 7.   984.837600  -0.057690   -0.005560    0.810600    c
|  8.     24.688260      24.688320      -0.000060     | 8.   984.779910  -0.069800   -0.012110    0.743200
|  9.     27.285136      27.285300      -0.000164     | 9.   984.710110  -0.074460   -0.004660    0.582200    c
| 10.     29.881445      29.881500      -0.000055     |10.   984.635650  -0.080000   -0.005540    0.800000
| 11.     32.477133      32.476720       0.000413     |11.   984.555650  -0.091380   -0.011380    0.687100
| 12.     35.072143      35.072030       0.000113     |12.   984.464270  -0.097650   -0.006270    0.705500    c
| 13.     37.666422      37.666500      -0.000078     |13.   984.366620  -0.107130   -0.009480    0.627200
| 14.     40.259914      40.260030      -0.000116     |14.   984.259490  -0.108830   -0.001700    0.831300
| 15.     42.852563      42.852630      -0.000067     |15.   984.150660  -0.119670   -0.010840    0.894300    c
| 16.     45.444315      45.444460      -0.000145     |16.   984.030990  -0.124000   -0.004330    0.792700    c
| 17.     48.035113      48.035950      -0.000837     |17.   983.906990  -0.131700   -0.007700    0.864800
| 18.     50.624902      50.625440      -0.000538     |18.   983.775290  -0.139220   -0.007520    0.698700
| 19.     53.213626      53.214230      -0.000604     |19.   983.636070  -0.145160   -0.005940    0.702000
| 20.     50.624902      55.801710      -0.000483     |20.   983.490910  -0.156330   -0.011170    0.760200    c
| 21.     58.387650      58.387950      -0.000300     |21.   983.334580  -0.152220    0.004110    0.781700    c
| 22.     55.801227                                   |22.   983.182360  -0.151280    0.000940    0.901200
| 23.     58.387650                                   |23.   983.031080  -0.167490   -0.016210    0.851200
| 24.     60.972838                                   |24.   982.863590                           0.847900
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K=5   n=1   A+

(125)A

R_branch

J	wv	delta1	delta2	intens	Comm
5.	992.666240	1.228480		0.908100	
6.	993.894720	1.220780	-0.007700	0.865300	c
7.	995.115500	1.213640	-0.007140	0.842000	c
8.	996.329140	1.207520	-0.006120	0.626000	c
9.	997.536660	1.199880	-0.007640	0.782700	c
10.	998.736540	1.192840	-0.007040	0.776500	c
11.	999.929380	1.185700	-0.007140	0.789600	c
12.	1001.115080	1.178640	-0.007060	0.773600	c
13.	1002.293720	1.171450	-0.007190	0.757400	
14.	1003.465170	1.164380	-0.007070	0.737500	c
15.	1004.629550	1.157290	-0.007090	0.768700	c
16.	1005.786840	1.150150	-0.007140	0.783800	c
17.	1006.936990	1.141530	-0.008620	0.749000	
18.	1008.078520	1.132630	-0.008900	0.600600	
19.	1009.211150	1.123770	-0.008860	0.784200	
20.	1010.334920	1.118340	-0.005430	0.823600	
21.	1011.453260	1.113040	-0.005300	0.741100	
22.	1012.566300	1.107450	-0.005590	0.679400	
23.	1013.673750	1.097440	-0.010010	0.643600	
24.	1014.771190	1.086140	-0.011300	0.687400	
25.	1015.857330	1.075380	-0.010760	0.898700	
26.	1016.932710			0.909200	

P_branch

J	wv	delta1	delta2	intens	Comm
6.	977.137180	-1.363970		0.856800	
7.	975.773210	-1.369940	-0.005970	0.842700	c
8.	974.403270	-1.376570	-0.006630	0.818900	c
9.	973.026700	-1.383230	-0.006660	0.834800	c
10.	971.643470	-1.389650	-0.006420	0.816700	c
11.	970.253820	-1.396090	-0.006440	0.745300	c
12.	968.857730	-1.402700	-0.006610	0.808100	c
13.	967.455030	-1.409050	-0.006350	0.798500	c
14.	966.045980	-1.415520	-0.006470	0.803100	
15.	964.630460	-1.421900	-0.006380	0.811700	c
16.	963.208560	-1.428170	-0.006270	0.822200	c
17.	961.780390	-1.434160	-0.005990	0.799400	c
18.	960.346230	-1.440730	-0.006570	0.821500	
19.	958.905500	-1.445930	-0.005200	0.705000	
20.	957.459570	-1.452500	-0.006570	0.841200	
21.	956.007070	-1.458180	-0.005680	0.856200	
22.	954.548890	-1.464090	-0.005910	0.853500	
23.	953.084800	-1.469870	-0.005780	0.879700	
24.	951.614930	-1.475350	-0.005480	0.887500	
25.	950.139580	-1.481100	-0.005750	0.900700	
26.	948.658480	-1.486590	-0.005490	0.908700	
27.	947.171890	-1.492140	-0.005550	0.924500	
28.	945.679750	-1.497310	-0.005170	0.929300	
29.	944.182440			0.921200	

(125)A

	RP_cal	RP_obs	diff
5.	16.893270	16.893030	0.000240
6.	19.491296	19.491450	-0.000154
7.	22.088919	22.088800	0.000119
8.	24.686086	24.685670	0.000416
9.	27.282741	27.282840	-0.000099
10.	29.878831	29.878810	0.000021
11.	32.474301	32.474350	-0.000049
12.	35.069098	35.069100	-0.000002
13.	37.663166	37.663260	-0.000094
14.	40.256449	40.256610	-0.000161
15.	42.848894	42.849160	-0.000266
16.	45.440445	45.440610	-0.000165
17.	48.031047	48.031490	-0.000443
18.	50.620643	50.618950	0.001693
19.	53.209177	53.204080	0.005097
20.	55.796595	55.786030	0.010565
21.	58.382839	58.368460	0.014379
22.	60.967853	60.951370	0.016483
23.	63.551580	63.534170	0.017410
24.	66.133962	66.112710	0.021252

Q_branch

J	wv	delta1	delta2	intens	Comm
5.	984.931730	-0.062470		0.273400	
6.	984.869260	-0.070960	-0.008490	0.436400	c
7.	984.798300	-0.078640	-0.007680	0.656000	c
8.	984.719660	-0.084010	-0.005370	0.743000	c
9.	984.635650	-0.090890	-0.006880	0.800000	c
10.	984.544760	-0.098680	-0.007790	0.589700	c
11.	984.446080	-0.105360	-0.006680	0.708000	c
12.	984.340720	-0.109340	-0.003980	0.728500	c
13.	984.231380	-0.119170	-0.009830	0.880000	
14.	984.112210	-0.127260	-0.008090	0.816400	c
15.	983.984950	-0.131850	-0.004590	0.646900	c
16.	983.853100	-0.138020	-0.006170	0.926900	c
17.	983.715080			0.868000	

K=0   n=1   E1   (130)E

R_branch

J	wv	delta1	delta2	intens	Comm
4.	991.472520	1.256910		0.795600	
5.	992.729430	1.248910	-0.008000	0.796900	c
6.	993.978340	1.241710	-0.007200	0.770300	c
7.	995.220050	1.234280	-0.007430	0.766600	
8.	996.454330	1.226920	-0.007360	0.729200	c
9.	997.681250	1.218560	-0.008360	0.722900	c
10.	998.899810	1.212730	-0.005830	0.662100	
11.	1000.112540	1.204580	-0.008150	0.739200	
12.	1001.317120	1.197180	-0.007400	0.734900	c
13.	1002.514300	1.189640	-0.007540	0.729900	
14.	1003.703940	1.182060	-0.007580	0.739200	
15.	1004.886000	1.174630	-0.007430	0.735700	
16.	1006.060630	1.167150	-0.007480	0.754800	
17.	1007.227780	1.159710	-0.007440	0.756700	
18.	1008.387490	1.152250	-0.007460	0.776000	
19.	1009.539740	1.144470	-0.007780	0.798500	
20.	1010.684210	1.136950	-0.007520	0.809100	
21.	1011.821160	1.129530	-0.007420	0.810400	
22.	1012.950690	1.121980	-0.007550	0.804900	
23.	1014.072670	1.114580	-0.007400	0.844500	
24.	1015.187250	1.107690	-0.006890	0.868900	
25.	1016.294940	1.098690	-0.009000	0.823800	
26.	1017.393630	1.091810	-0.006880	0.835500	
27.	1018.485440	1.084080	-0.007730	0.908600	
28.	1019.569520	1.073870	-0.010210	0.901400	
29.	1020.643390	1.071330	-0.002540	0.870600	
30.	1021.714720	1.068230	-0.003100	0.912700	
31.	1022.782950	1.062220	-0.006010	0.864700	
32.	1023.845170			0.870100	

P_branch

J	wv	delta1	delta2	intens	Comm
1.	983.781440	-1.306770		0.884300	
2.	982.474670	-1.314250	-0.007480	0.890900	
3.	981.160420	-1.320960	-0.006710	0.884700	
4.	979.839460	-1.328770	-0.007810	0.822000	
5.	978.510690	-1.336000	-0.007230	0.756900	
6.	977.174690	-1.342270	-0.006270	0.692900	c
7.	975.832420	-1.349620	-0.007350	0.788000	c
8.	974.482800	-1.356400	-0.006780	0.776700	
9.	973.126400	-1.363390	-0.006990	0.767200	c
10.	971.763010	-1.370310	-0.006920	0.764100	c
11.	970.392700	-1.377060	-0.006750	0.690600	
12.	969.015640	-1.383890	-0.006830	0.760200	
13.	967.631750	-1.390450	-0.006560	0.761300	c
14.	966.241300	-1.397500	-0.007050	0.539300	
15.	964.843800	-1.403900	-0.006400	0.753300	
16.	963.439900	-1.410680	-0.006780	0.772600	
17.	962.029220	-1.416710	-0.006030	0.751500	
18.	960.612510	-1.424130	-0.007420	0.768700	
19.	959.188380	-1.430070	-0.005940	0.810800	
20.	957.758310	-1.436720	-0.006650	0.814600	
21.	956.321590	-1.442860	-0.006140	0.806200	
22.	954.878730	-1.449310	-0.006450	0.842400	
23.	953.429420	-1.455570	-0.006260	0.848300	
24.	951.973850	-1.461760	-0.006190	0.864600	
25.	950.512090	-1.468140	-0.006380	0.880300	
26.	949.043950	-1.473930	-0.005790	0.891500	
27.	947.570020	-1.479980	-0.006050	0.899600	
28.	946.090040	-1.486880	-0.006900	0.895400	
29.	944.603160			0.889900	

(130)E1

					Q_branch				
	RP_cal	RP_obs	diff	J	wv	delta1	delta2	intens	Comm
4.	14.298044	14.297830	0.000214						
5.	16.896957	16.897010	-0.000053	5.	984.972240	-0.040510		0.614800	c
6.	19.495505	19.495540	-0.000035	6.	984.931730	-0.052600	-0.012090	0.273400	c
7.	22.093631	22.093650	-0.000019	7.	984.879130	-0.057730	-0.005130	0.777700	
8.	24.691277	24.691320	-0.000043	8.	984.821400	-0.062760	-0.005030	0.756100	c
9.	27.288388	27.288550	-0.000162	9.	984.758640	-0.072580	-0.009820	0.744400	c
10.	29.884907	29.884170	0.000737	10.	984.686060	-0.082610	-0.010030	0.880000	
11.	32.480778	32.480790	-0.000012	11.	984.603450	-0.081550	0.001060	0.883700	
12.	35.075941	35.075820	0.000121	12.	984.521900	-0.094640	-0.013090	0.818800	c
13.	37.670340	37.670500	-0.000160	13.	984.427260			0.807700	
14.	40.263919	40.264040	-0.000121						
15.	42.856619	42.856780	-0.000161						
16.	45.448382	45.448120	0.000262						
17.	48.039151	48.039400	-0.000249						
18.	50.628867	50.629180	-0.000313						
19.	53.217472	53.218150	-0.000678						
20.	55.804908	55.805480	-0.000572						
21.	58.391115	58.391740	-0.000625						
22.	60.976033	60.976840	-0.000807						
23.	63.559604	63.560580	-0.000976						
24.	66.141768	66.143300	-0.001532						
25.									
26.									
27.									
28.									
29.									
30.									
31.									
32.									

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K=1    n=1    A+                                                        (131)A+

 R_branch                                                              |  P_branch

  J          wv          delta1       delta2        intens    Comm     |    J          wv          delta1       delta2        intens    Comm
  1.     987.213000   1.269990                   0.901500              |
  2.     988.482990   1.267850   -0.002140    0.921700              |    2.     982.025180   -1.314210                  0.920300
  3.     989.750840   1.259960   -0.007890    0.899100              |    3.     980.710970   -1.321380   -0.007170    0.852300
  4.     991.010800   1.252120   -0.007840    0.872300              |    4.     979.389590   -1.330330   -0.008950    0.822500
  5.     992.262920   1.243710   -0.008410    0.860800              |    5.     978.059260   -1.337690   -0.007360    0.865800
  6.     993.506630   1.236600   -0.007110    0.697800              |    6.     976.721570   -1.345370   -0.007680    0.873800
  7.     994.743230   1.228060   -0.008540    0.827900              |    7.     975.376200   -1.352860   -0.007490    0.853700
  8.     995.971290   1.220280   -0.007780    0.825800              |    8.     974.023340   -1.360360   -0.007500    0.844400
  9.     997.191570   1.212160   -0.008120    0.815600              |    9.     972.662980   -1.367820   -0.007460    0.828500
 10.     998.403730   1.204470   -0.007690    0.800000              |   10.     971.295160   -1.375180   -0.007360    0.828400
 11.     999.608200   1.196180   -0.008290    0.798400              |   11.     969.919980   -1.382800   -0.007620    0.818200
 12.    1000.804380   1.188540   -0.007640    0.677500              |   12.     968.537180   -1.389750   -0.006950    0.825100
 13.    1001.992920   1.178760   -0.009780    0.778800              |   13.     967.147430   -1.397350   -0.007600    0.777700
 14.    1003.171680   1.173990   -0.004770    0.480500              |   14.     965.750080   -1.404450   -0.007100    0.820200
 15.    1004.345670   1.164360   -0.009630    0.806400              |   15.     964.345630   -1.411450   -0.007000    0.828600
 16.    1005.510030   1.156310   -0.008050    0.367500              |   16.     962.934180   -1.418780   -0.007330    0.818500
 17.    1006.666340   1.148870   -0.007440    0.403900              |   17.     961.515400   -1.425620   -0.006840    0.830700
 18.    1007.815210   1.140670   -0.008200    0.823700              |   18.     960.089780   -1.432800   -0.007180    0.831700
 19.    1008.955880   1.134780   -0.005890    0.842000              |   19.     958.656980   -1.439600   -0.006800    0.820600
 20.    1010.090660   1.122630   -0.012150    0.685500              |   20.     957.217380   -1.446520   -0.006920    0.864700
 21.    1011.213290   1.116900   -0.005730    0.866600              |   21.     955.770860   -1.452890   -0.006370    0.831000
 22.    1012.330190   1.108750   -0.008150    0.876100              |   22.     954.317970   -1.460520   -0.007630    0.829600
 23.    1013.438940   1.101250   -0.007500    0.863500              |   23.     952.857450   -1.474420   -0.013900    0.889800
 24.    1014.540190   1.091560   -0.009690    0.890500              |   24.     951.383030                              0.893200
 25.    1015.631750   1.087050   -0.004510    0.890000              |
 26.    1016.718800   1.078740   -0.008310    0.923400              |
 27.    1017.797540   1.073210   -0.005530    0.930300              |
 28.    1018.870750   1.067790   -0.005420    0.966300              |
 29.    1019.938540                          0.875500              |
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                                  (131)A+

|                                            |     Q_branch
|         RP_cal        RP_obs         diff  | J        wv         delta1       delta2      intens   Comm
|  1.     6.495698      6.502030    -0.006332 |
|  2.     9.093781      9.093400     0.000381 |
|  3.    11.691665     11.691580     0.000085 |
|  4.    14.289295     14.289230     0.000065 |
|  5.    16.886615     16.886720    -0.000105 |
|  6.    19.483567     19.483290     0.000277 |
|  7.    22.080096     22.080250    -0.000154 |
|  8.    24.676145     24.676130     0.000015 |
|  9.    27.271656     27.271590     0.000066 |
| 10.    29.866571     29.866550     0.000021 |
| 11.    32.460835     32.460770     0.000065 |
| 12.    35.054390     35.054300     0.000090 |12.   983.906990  -0.119700                 0.864800
| 13.    37.647178     37.647290    -0.000112 |13.   983.787290  -0.129770   -0.010070    0.926500
| 14.    40.239143     40.237500     0.001643 |14.   983.657520  -0.139860   -0.010090    0.870900
| 15.    42.830224     42.830270    -0.000046 |15.   983.517660  -0.147750   -0.007890    0.863700
| 16.    45.420366     45.420250     0.000116 |16.   983.369910  -0.156510   -0.008760    0.809800
| 17.    48.009510     48.009360     0.000150 |17.   983.213400  -0.165230   -0.008720    0.727300
| 18.    50.597596     50.597830    -0.000234 |18.   983.048170  -0.172000   -0.006770    0.835700
| 19.    53.184569     53.185020    -0.000451 |19.   982.876170  -0.182930   -0.010930    0.910600
| 20.    55.770367     55.772690    -0.002323 |20.   982.693240                            0.727400
| 21.    58.354931     58.355840    -0.000909 |
| 22.    60.938204     60.947160    -0.008956 |
| 23.                                        |
| 24.                                        |
| 25.                                        |
| 26.                                        |
| 27.                                        |
| 28.                                        |
| 29.                                        |
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K=1    n=1    A-                                  (131)A-

  R_branch                                             |  P_branch

 J      wv        delta1      delta2    intens   Comm  |   J      wv        delta1     delta2     intens   Comm
 1.  987.213000  1.281470             0.901500       |
 2.  988.494470  1.273860  -0.007610  0.925200       |   2. 982.025180  -1.314210             0.920300
 3.  989.768330  1.267120  -0.006740  0.902300       |   3. 980.710970  -1.321380  -0.007170  0.852300
 4.  991.035450  1.260330  -0.006790  0.880100       |   4. 979.389590  -1.326590  -0.005210  0.822500
 5.  992.295780  1.253470  -0.006860  0.857200       |   5. 978.063000  -1.333710  -0.007120  0.868800
 6.  993.549250  1.246820  -0.006650  0.836700       |   6. 976.729290  -1.340060  -0.006350  0.874900
 7.  994.796070  1.239630  -0.007190  0.822200       |   7. 975.389230  -1.346360  -0.006300  0.853800
 8.  996.035700  1.233060  -0.006570  0.811900       |   8. 974.042870  -1.353140  -0.006780  0.843900
 9.  997.268760  1.226060  -0.007000  0.793500       |   9. 972.689730  -1.359340  -0.006200  0.823200
10.  998.494820  1.219280  -0.006780  0.709800       |  10. 971.330390  -1.365320  -0.005980  0.737800
11.  999.714100  1.212140  -0.007140  0.693800       |  11. 969.965070  -1.371810  -0.006490  0.815800
12. 1000.926240  1.205460  -0.006680  0.794400       |  12. 968.593260  -1.378110  -0.006300  0.814600
13. 1002.131700  1.198390  -0.007070  0.809100       |  13. 967.215150  -1.383910  -0.005800  0.806600
14. 1003.330090  1.191660  -0.006730  0.816100       |  14. 965.831240  -1.391260  -0.007350  0.819200
15. 1004.521750  1.184370  -0.007290  0.807300       |  15. 964.439980  -1.396050  -0.004790  0.733900
16. 1005.706120  1.177430  -0.006940  0.722900       |  16. 963.043930  -1.402470  -0.006420  0.835800
17. 1006.883550  1.170770  -0.006660  0.688600       |  17. 961.641460  -1.408530  -0.006060  0.844700
18. 1008.054320  1.162890  -0.007880  0.805600       |  18. 960.232930  -1.414590  -0.006060  0.831200
19. 1009.217210  1.156430  -0.006460  0.728300       |  19. 958.818340  -1.420500  -0.005910  0.854600
20. 1010.373640  1.150570  -0.005860  0.702600       |  20. 957.397840  -1.426190  -0.005690  0.860200
21. 1011.524210  1.142660  -0.007910  0.843700       |  21. 955.971650  -1.432210  -0.006020  0.871400
22. 1012.666870  1.135530  -0.007130  0.869800       |  22. 954.539440  -1.437930  -0.005720  0.887400
23. 1013.802400  1.128630  -0.006900  0.900200       |  23. 953.101510  -1.443480  -0.005550  0.886500
24. 1014.931030  1.121120  -0.007510  0.891100       |  24. 951.658030  -1.449380  -0.005900  0.889000
25. 1016.052150  1.114950  -0.006170  0.791300       |  25. 950.208650  -1.454830  -0.005450  0.906000
26. 1017.167100  1.108710  -0.006240  0.808400       |  26. 948.753820  -1.460460  -0.005630  0.912400
27. 1018.275810  1.100140  -0.008570  0.858500       |  27. 947.293360  -1.465760  -0.005300  0.921000
28. 1019.375950  1.095060  -0.005080  0.841400       |  28. 945.827600  -1.471600  -0.005840  0.940100
29. 1020.471010  1.090220  -0.004840  0.933000       |  29. 944.356000  -1.476330  -0.004730  0.942500
30. 1021.561230  1.084810  -0.005410  0.939300       |  30. 942.879670                        0.949600
31. 1022.646040  1.079870  -0.004940  0.865900       |
32. 1023.725910                       0.886900       |
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                                   (131)A-

|                                          !     Q_branch

|          RP_cal      RP_obs      diff    | J      wv        delta1      delta2     intens   Comm
|  1.     6.503375    6.502030    0.001345 |
|  2.     9.104524    9.104880   -0.000356 | 2.  984.619070  -0.015620               0.796200
|  3.    11.705471   11.705330    0.000141 | 3.  984.603450  -0.021410  -0.005790   0.883700
|  4.    14.306158   14.306160   -0.000002 | 4.  984.582040  -0.026390  -0.004980   0.657700
|  5.    16.906528   16.906550   -0.000022 | 5.  984.555650  -0.033750  -0.007360   0.687100
|  6.    19.506523   19.506380    0.000143 | 6.  984.521900  -0.034860  -0.001110   0.818800
|  7.    22.106087   22.106340   -0.000253 | 7.  984.487040  -0.040960  -0.006100   0.718400
|  8.    24.705158   24.705310   -0.000152 | 8.  984.446080  -0.045170  -0.004210   0.708000
|  9.    27.303680   27.303690   -0.000010 | 9.  984.400910  -0.048330  -0.003160   0.829900
| 10.    29.901596   29.901560    0.000036 |10.  984.352580  -0.058210  -0.009880   0.763300
| 11.    32.498845   32.498950   -0.000105 |11.  984.294370  -0.062990  -0.004780   0.743700
| 12.    35.095371   35.095000    0.000371 |12.  984.231380  -0.065050  -0.002060   0.880000
| 13.    37.691113   37.691720   -0.000607 |13.  984.166330  -0.070980  -0.005930   0.713400
| 14.    40.286014   40.286160   -0.000146 |14.  984.095350                         0.889200
| 15.    42.880015   42.880290   -0.000275 |
| 16.    45.473055   45.473190   -0.000135 |
| 17.    48.065076   48.065210   -0.000134 |
| 18.    50.656018   50.656480   -0.000462 |
| 19.    53.245823   53.245560    0.000263 |
| 20.    55.834429   55.834200    0.000229 |
| 21.    58.421776   58.422700   -0.000924 |
| 22.    61.007805   61.008840   -0.001035 |
| 23.    63.592454   63.593750   -0.001296 |
| 24.    66.175664   66.177210   -0.001546 |
| 25.                                      |
| 26.                                      |
| 27.                                      |
| 28.                                      |
| 29.                                      |
| 30.                                      |
| 31.                                      |
| 32.                                      |
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K=2    n=1    E2                                                    (132)E2

  R_branch                                                       |  P_branch

 J          wv        delta1       delta2       intens    Comm   |    J         wv         delta1        delta2       intens    Comm
 2.    989.887530   1.279560                  0.943800           |
 3.    991.167090   1.265360   -0.014200     0.909100           |    3.    982.117200   -1.320560                   0.915400
 4.    992.432450   1.258330   -0.007030     0.891700           |    4.    980.796640   -1.327430   -0.006870      0.907000
 5.    993.690780   1.251100   -0.007230     0.861000           |    5.    979.469210   -1.333830   -0.006400      0.858300
 6.    994.941880   1.243780   -0.007320     0.830000           |    6.    978.135380   -1.340650   -0.006820      0.879000
 7.    996.185660   1.237360   -0.006420     0.842700           |    7.    976.794730   -1.347170   -0.006520      0.867200
 8.    997.423020   1.229910   -0.007450     0.843200           |    8.    975.447560   -1.353760   -0.006590      0.857700
 9.    998.652930   1.223360   -0.006550     0.756400           |    9.    974.093800   -1.360800   -0.007040      0.816100
10.    999.876290   1.216120   -0.007240     0.807200           |   10.    972.733000   -1.366240   -0.005440      0.707500
11.   1001.092410   1.209250   -0.006870     0.817600           |   11.    971.366760   -1.372860   -0.006620      0.820800
12.   1002.301660   1.202340   -0.006910     0.815400           |   12.    969.993900   -1.379450   -0.006590      0.815900
13.   1003.504000   1.195310   -0.007030     0.807000           |   13.    968.614450   -1.385290   -0.005840      0.835500
14.   1004.699310   1.188280   -0.007030     0.791800           |   14.    967.229160   -1.392250   -0.006960      0.763300
15.   1005.887590   1.181650   -0.006630     0.813200           |   15.    965.836910   -1.396930   -0.004680      0.843200
16.   1007.069240   1.174700   -0.006950     0.834500           |   16.    964.439980   -1.404690   -0.007760      0.733900
17.   1008.243940   1.168200   -0.006500     0.845000           |   17.    963.035290   -1.409840   -0.005150      0.849800
18.   1009.412140   1.160100   -0.008100     0.841800           |   18.    961.625450   -1.415560   -0.005720      0.861900
19.   1010.572240   1.156900   -0.003200     0.872500           |   19.    960.209890   -1.420960   -0.005400      0.856300
20.   1011.729140   1.147900   -0.009000     0.817000           |   20.    958.788930   -1.428020   -0.007060      0.884800
21.   1012.877040   1.143480   -0.004420     0.815600           |   21.    957.360910   -1.431260   -0.003240      0.879700
22.   1014.020520   1.131960   -0.011520     0.636500           |   22.    955.929650   -1.438010   -0.006750      0.886800
23.   1015.152480   1.117510   -0.014450     0.899000           |   23.    954.491640   -1.442550   -0.004540      0.881700
24.   1016.269990                            0.938000           |   24.    953.049090   -1.447960   -0.005410      0.921200
                                                                 |   25.    951.601130   -1.453140   -0.005180      0.922200
                                                                 |   26.    950.147990   -1.457430   -0.004290      0.931600
                                                                 |   27.    948.690560   -1.462740   -0.005310      0.923000
                                                                 |   28.    947.227820                              0.929500
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(132)E2

```
|                                                 Q_branch
|         RP_cal       RP_obs        diff     | J       wv       delta1     delta2     intens   Comm
|  1.                                         |
|  2.     9.098771     9.090890    0.007881   |
|  3.    11.698070    11.697880    0.000190   |
|  4.    14.297104    14.297070    0.000034   |
|  5.    16.895818    16.896050   -0.000232   |
|  6.    19.494151    19.494320   -0.000169   |
|  7.    22.092044    22.091860    0.000184   |
|  8.    24.689440    24.690020   -0.000580   |
|  9.    27.286279    27.286170    0.000109   |
| 10.    29.882501    29.882390    0.000111   |
| 11.    32.478048    32.477960    0.000088   |
| 12.    35.072862    35.072500    0.000362   |
| 13.    37.666881    37.667090   -0.000209   |
| 14.    40.260047    40.259330    0.000717   |
| 15.    42.852299    42.852300   -0.000001   |
| 16.    45.443577    45.443790   -0.000213   |
| 17.    48.033824    48.034050   -0.000226   |
| 18.    50.622977    50.623210   -0.000233   |
| 19.    53.210975    53.211330   -0.000355   |
| 20.    55.797759    55.799490   -0.001731   |
| 21.    58.383269    58.385400   -0.002131   |
| 22.    60.967444    60.971430   -0.003986   |
| 23.    63.550222    63.551350   -0.001128   |
| 24.    66.131542    66.122000    0.009542   |
|                                             |
|                                             |
|                                             |
|                                             |
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K=3   n=1   E1                                                     (133)E1

 R_branch                                                         |  P_branch

 J         wv         delta1      delta2      intens   Comm       |   J        wv         delta1      delta2      intens   Comm
 3.     989.101140   1.262740                0.923900   c         |
 4.     990.363880   1.255010   -0.007730   0.861900   c         |   4.    978.733350  -1.329300               0.931400    c
 5.     991.618890   1.247210   -0.007800   0.836700             |   5.    977.404050  -1.336420  -0.007120   0.886400    c
 6.     992.866100   1.240080   -0.007130   0.793300   c         |   6.    976.067630  -1.343550  -0.007130   0.846200
 7.     994.106180   1.232010   -0.008070   0.766200   c         |   7.    974.724080  -1.350720  -0.007170   0.841700    c
 8.     995.338190   1.224700   -0.007310   0.774400   c         |   8.    973.373360  -1.357730  -0.007010   0.813000    c
 9.     996.562890   1.217610   -0.007090   0.757400             |   9.    972.015630  -1.364860  -0.007130   0.785500    c
10.     997.780500   1.208780   -0.008830   0.613700             |  10.    970.650770  -1.372010  -0.007150   0.757500
11.     998.989280   1.201910   -0.006870   0.722900             |  11.    969.278760  -1.378850  -0.006840   0.760700
12.    1000.191190   1.194170   -0.007740   0.747100             |  12.    967.899910  -1.385800  -0.006950   0.766100
13.    1001.385360   1.186550   -0.007620   0.753500             |  13.    966.514110  -1.392550  -0.006750   0.767400
14.    1002.571910   1.178870   -0.007680   0.744900             |  14.    965.121560  -1.400060  -0.007510   0.779200
15.    1003.750780   1.172010   -0.006860   0.750300             |  15.    963.721500  -1.405490  -0.005430   0.650000
16.    1004.922790   1.163120   -0.008890   0.701500             |  16.    962.316010  -1.412640  -0.007150   0.783200
17.    1006.085910   1.156070   -0.007050   0.761000             |  17.    960.903370  -1.419530  -0.006890   0.766300
18.    1007.241980   1.148570   -0.007500   0.746300             |  18.    959.483840  -1.425950  -0.006420   0.800000
19.    1008.390550   1.140870   -0.007700   0.789100             |  19.    958.057890  -1.432880  -0.006930   0.796300
20.    1009.531420   1.133230   -0.007640   0.802300             |  20.    956.625010  -1.438410  -0.005530   0.728300
21.    1010.664650   1.125790   -0.007440   0.825600             |  21.    955.186600  -1.445110  -0.006700   0.830800
22.    1011.790440   1.118110   -0.007680   0.841200             |  22.    953.741490  -1.451730  -0.006620   0.834800
23.    1012.908550   1.111970   -0.006140   0.849500             |  23.    952.289760  -1.457370  -0.005640   0.822800
24.    1014.020520   1.101730   -0.010240   0.636500             |  24.    950.832390  -1.463660  -0.006290   0.808800
25.    1015.122250   1.095970   -0.005760   0.882900             |  25.    949.368730  -1.470240  -0.006580   0.754100
26.    1016.218220   1.087520   -0.008450   0.799500             |  26.    947.898490  -1.476070  -0.005830   0.892600
27.    1017.305740   1.080660   -0.006860   0.899000             |  27.    946.422420  -1.481810  -0.005740   0.902800
28.    1018.386400   1.072950   -0.007710   0.801800             |  28.    944.940610  -1.487800  -0.005990   0.916500
29.    1019.459350   1.065180   -0.007770   0.898600             |  29.    943.452810  -1.493520  -0.005720   0.930800
30.    1020.524530   1.058030   -0.007150   0.918500             |  30.    941.959290  -1.499350  -0.005830   0.930400
31.    1021.582560   1.052780   -0.005250   0.946300             |  31.    940.459940  -1.504800  -0.005450   0.942100
32.    1022.635340   1.046990   -0.005790   0.808700             |  32.    938.955140  -1.510960  -0.006160   0.921100
33.    1023.682330                           0.952500             |  33.    937.444180                          0.961200
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                                   (133)E1

|                                                       Q_branch

|         RP_cal       RP_obs          diff     | J        wv       delta1      delta2      intens   Comm
|  3.   11.697330    11.697090     0.000240     | 3.  983.931970  -0.029450               0.494900    c
|  4.   14.296173    14.296250    -0.000077     | 4.  983.902520  -0.038510   -0.009060   0.779200    c
|  5.   16.894678    16.894810    -0.000132     | 5.  983.864010  -0.044170   -0.005660   0.690100
|  6.   19.492782    19.492740     0.000042     | 6.  983.819840  -0.050410   -0.006240   0.648200    c
|  7.   22.090423    22.090550    -0.000127     | 7.  983.769430  -0.059940   -0.009530   0.845600    c
|  8.   24.687541    24.687420     0.000121     | 8.  983.709490  -0.065580   -0.005640   0.701100    c
|  9.   27.284073    27.284130    -0.000057     | 9.  983.643910  -0.071080   -0.005500   0.799800
| 10.   29.879957    29.880590    -0.000633     |10.  983.572830  -0.081920   -0.010840   0.764100
| 11.   32.475132    32.475170    -0.000038     |11.  983.490910  -0.090220   -0.008300   0.760200
| 12.   35.069534    35.069630    -0.000096     |12.  983.400690  -0.091060   -0.000840   0.948200
| 13.   37.663102    37.663860    -0.000758     |13.  983.309630  -0.091790   -0.000730   0.753500
| 14.   40.255773    40.255900    -0.000127     |14.  983.217840  -0.093490   -0.001700   0.813700
| 15.   42.847485    42.847410     0.000075     |15.  983.124350  -0.102080   -0.008590   0.834800
| 16.   45.438176    45.438950    -0.000774     |16.  983.022270  -0.110470   -0.008390   0.917100
| 17.   48.027782    48.028020    -0.000238     |17.  982.911800  -0.118630   -0.008160   0.799800
| 18.   50.616241    50.616970    -0.000729     |18.  982.793170                          0.945300
| 19.   53.203491    53.203950    -0.000459     |
| 20.   55.789469    55.789930    -0.000461     |
| 21.   58.374112    58.374890    -0.000778     |
| 22.   60.957358    60.958050    -0.000692     |
| 23.   63.539145    63.539820    -0.000675     |
| 24.   66.119409    66.122030    -0.002621     |
| 25.                                           |
| 26.                                           |
| 27.                                           |
| 28.                                           |
| 29.                                           |
| 30.                                           |
| 31.                                           |
| 32.                                           |
| 33.                                           |
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K=4    n=1    A+                                                (134)A

 R_branch                                                      |  P_branch

 J          wv        delta1      delta2       intens    Comm  |    J          wv        delta1      delta2       intens    Comm
 4.    990.133870   1.254340                  0.918800    c    |
 5.    991.388210   1.246690   -0.007650     0.856200    c    |    5.    977.174690   -1.335470                  0.692900    c
 6.    992.634900   1.238980   -0.007710     0.818400    c    |    6.    975.839220   -1.344040   -0.008570     0.871200    c
 7.    993.873880   1.231420   -0.007560     0.772900    c    |    7.    974.495180   -1.351060   -0.007020     0.823700    c
 8.    995.105300   1.223840   -0.007580     0.738400    c    |    8.    973.144120   -1.358300   -0.007240     0.770800    c
 9.    996.329140   1.215400   -0.008440     0.626000         |    9.    971.785820   -1.365230   -0.006930     0.730400    c
10.    997.544540   1.208490   -0.006910     0.492400         |   10.    970.420590   -1.372420   -0.007190     0.731000
11.    998.753030   1.200430   -0.008060     0.708400         |   11.    969.048170   -1.379460   -0.007040     0.739900
12.    999.953460   1.192790   -0.007640     0.678300         |   12.    967.668710   -1.386370   -0.006910     0.741300
13.   1001.146250   1.185160   -0.007630     0.635100         |   13.    966.282340   -1.393470   -0.007100     0.730200
14.   1002.331410   1.177370   -0.007790     0.694400         |   14.    964.888870   -1.399850   -0.006380     0.497600
15.   1003.508780   1.169560   -0.007810     0.698700         |   15.    963.489020   -1.406870   -0.007020     0.734900
16.   1004.678340   1.161850   -0.007710     0.718500         |   16.    962.082150   -1.413470   -0.006600     0.725700
17.   1005.840190   1.154280   -0.007570     0.715100         |   17.    960.668680   -1.420240   -0.006770     0.740600
18.   1006.994470   1.146510   -0.007770     0.736400         |   18.    959.248440   -1.426650   -0.006410     0.761200
19.   1008.140980   1.138570   -0.007940     0.740100         |   19.    957.821790   -1.432720   -0.006070     0.757600
20.   1009.279550   1.131260   -0.007310     0.767000         |   20.    956.389070   -1.441130   -0.008410     0.666800
21.   1010.410810   1.123380   -0.007880     0.787500         |   21.    954.947940   -1.444900   -0.003770     0.742800
22.   1011.534190   1.116760   -0.006620     0.809300         |   22.    953.503040   -1.452870   -0.007970     0.803600
23.   1012.650950   1.106960   -0.009800     0.545800         |   23.    952.050170   -1.458300   -0.005430     0.794800
24.   1013.757910   1.100290   -0.006670     0.837700         |   24.    950.591870   -1.464430   -0.006130     0.824500
25.   1014.858200   1.092890   -0.007400     0.819000         |   25.    949.127440   -1.470870   -0.006440     0.839600
26.   1015.951090   1.088990   -0.003900     0.866900         |   26.    947.656570   -1.476780   -0.005910     0.871900
27.   1017.040080   1.073960   -0.015030     0.687000         |   27.    946.179790   -1.482590   -0.005810     0.883700
28.   1018.114040   1.063700   -0.010260     0.886700         |   28.    944.697200   -1.488620   -0.006030     0.901800
29.   1019.177740   1.057860   -0.005840     0.946900         |   29.    943.208580   -1.494280   -0.005660     0.917000
30.   1020.235600                             0.803900         |   30.    941.714300   -1.499810   -0.005530     0.920400
                                                               |   31.    940.214490                             0.924700
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(134)A

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|                                                           |        Q_branch
|            RP_cal        RP_obs         diff              | J          wv          delta1       delta2       intens    Comm
|  4.     14.294788     14.294650      0.000138             | 4.    983.672990  -0.036920                   0.559200    c
|  5.     16.892974     16.893030     -0.000056             | 5.    983.636070  -0.044870   -0.007950     0.702000    c
|  6.     19.490726     19.490780     -0.000054             | 6.    983.591200  -0.052690   -0.007820     0.734400    c
|  7.     22.087976     22.088060     -0.000084             | 7.    983.538510  -0.059850   -0.007160     0.770200    c
|  8.     24.684659     24.684710     -0.000051             | 8.    983.478660  -0.066820   -0.006970     0.707300    c
|  9.     27.280708     27.280970     -0.000262             | 9.    983.411840  -0.077260   -0.010440     0.721600
| 10.     29.876055     29.875830      0.000225             |10.    983.334580  -0.079420   -0.002160     0.781700
| 11.     32.470635     32.470690     -0.000055             |11.    983.255160                            0.744800
| 12.     35.064380     35.064590     -0.000210             |
| 13.     37.657221     37.657230     -0.000009             |
| 14.     40.249095     40.249260     -0.000165             |
| 15.     42.839935     42.840100     -0.000165             |
| 16.     45.429672     45.429900     -0.000228             |
| 17.     48.018240     48.018400     -0.000160             |
| 18.     50.605575     50.605400      0.000175             |
| 19.     53.191611     53.193040     -0.001429             |
| 20.     55.776280     55.776510     -0.000230             |
| 21.     58.359519     58.360640     -0.001121             |
| 22.     60.941265     60.942320     -0.001055             |
| 23.     63.521450     63.523510     -0.002060             |
| 24.     66.100013     66.101340     -0.001327             |
| 25.                                                       |
| 26.                                                       |
| 27.                                                       |
| 28.                                                       |
| 29.                                                       |
| 30.                                                       |
|                                                           |
```

C.3 Samples of unsuccessful series assignments in the spectrum of CD_3OH in the 910-1300 cm^{-1} region.

This appendix gives the unsuccessful series (123)E2 assignments by MOSAA. (n τ K) and asymmetry values found for this series are wrong while R(3) through R(27) found are correct. One of the 'Three Line Group' R(4) 991.472520 is overlapped[2], which causes MOSAA to pick a wrong R-P combination difference (n=1, K=2, A+ series). The wrong R-P combination differences picked are very close to the R-P combination differences of (123)E2 in the first several Js, which lets MOSAA produce a correct P branch (P(4) through P(24) are right) in the result.

---

[2] which causes quite quite a large amount of bias in $\Delta 2$ as shown in the output.

```
K=2    n=1    E2                                     (1x2)E2

  R_branch                                                  |  P_branch

  J        wv        delta1     delta2      intens    Comm  |    J        wv       delta1      delta2      intens    Comm
  2.    989.887530   1.279560               0.943800        |
  3.    991.167090   1.265360   -0.014200   0.909100        |    3.   982.117200   -1.320560               0.915400
  4.    992.432450   1.258330   -0.007030   0.891700        |    4.   980.796640   -1.327430   -0.006870   0.907000
  5.    993.690780   1.251100   -0.007230   0.861000        |    5.   979.469210   -1.333830   -0.006400   0.858300
  6.    994.941880   1.243780   -0.007320   0.830000        |    6.   978.135380   -1.340650   -0.006820   0.879000
  7.    996.185660   1.237360   -0.006420   0.842700        |    7.   976.794730   -1.347170   -0.006520   0.867200
  8.    997.423020   1.229910   -0.007450   0.843200        |    8.   975.447560   -1.353760   -0.006590   0.857700
  9.    998.652930   1.223360   -0.006550   0.756400        |    9.   974.093800   -1.360800   -0.007040   0.816100
 10.    999.876290   1.216120   -0.007240   0.807200        |   10.   972.733000   -1.366240   -0.005440   0.707500
 11.   1001.092410   1.209250   -0.006870   0.817600        |   11.   971.366760   -1.372860   -0.006620   0.820800
 12.   1002.301660   1.202340   -0.006910   0.815400        |   12.   969.993900   -1.379450   -0.006590   0.815900
 13.   1003.504000   1.195310   -0.007030   0.807000        |   13.   968.614450   -1.385290   -0.005840   0.835500
 14.   1004.699310   1.188280   -0.007030   0.791800        |   14.   967.229160   -1.392250   -0.006960   0.763300
 15.   1005.887590   1.181650   -0.006630   0.813200        |   15.   965.836910   -1.396930   -0.004680   0.843200
 16.   1007.069240   1.174700   -0.006950   0.834500        |   16.   964.439980   -1.404690   -0.007760   0.733900
 17.   1008.243940   1.168200   -0.006500   0.845000        |   17.   963.035290   -1.409840   -0.005150   0.849800
 18.   1009.412140   1.160100   -0.008100   0.841800        |   18.   961.625450   -1.415560   -0.005720   0.861900
 19.   1010.572240   1.156900   -0.003200   0.872500        |   19.   960.209890   -1.420960   -0.005400   0.856300
 20.   1011.729140   1.147900   -0.009000   0.817000        |   20.   958.788930   -1.428020   -0.007060   0.884800
 21.   1012.877040   1.143480   -0.004420   0.815600        |   21.   957.360910   -1.431260   -0.003240   0.879700
 22.   1014.020520   1.131960   -0.011520   0.636500        |   22.   955.929650   -1.438010   -0.006750   0.886800
 23.   1015.152480   1.117510   -0.014450   0.899000        |   23.   954.491640   -1.442550   -0.004540   0.881700
 24.   1016.269990                          0.938000        |   24.   953.049090   -1.447960   -0.005410   0.921200
                                                            |   25.   951.601130   -1.453140   -0.005180   0.922200
                                                            |   26.   950.147990   -1.457430   -0.004290   0.931600
                                                            |   27.   948.690560   -1.462740   -0.005310   0.923000
                                                            |   28.   947.227820                           0.929500
```

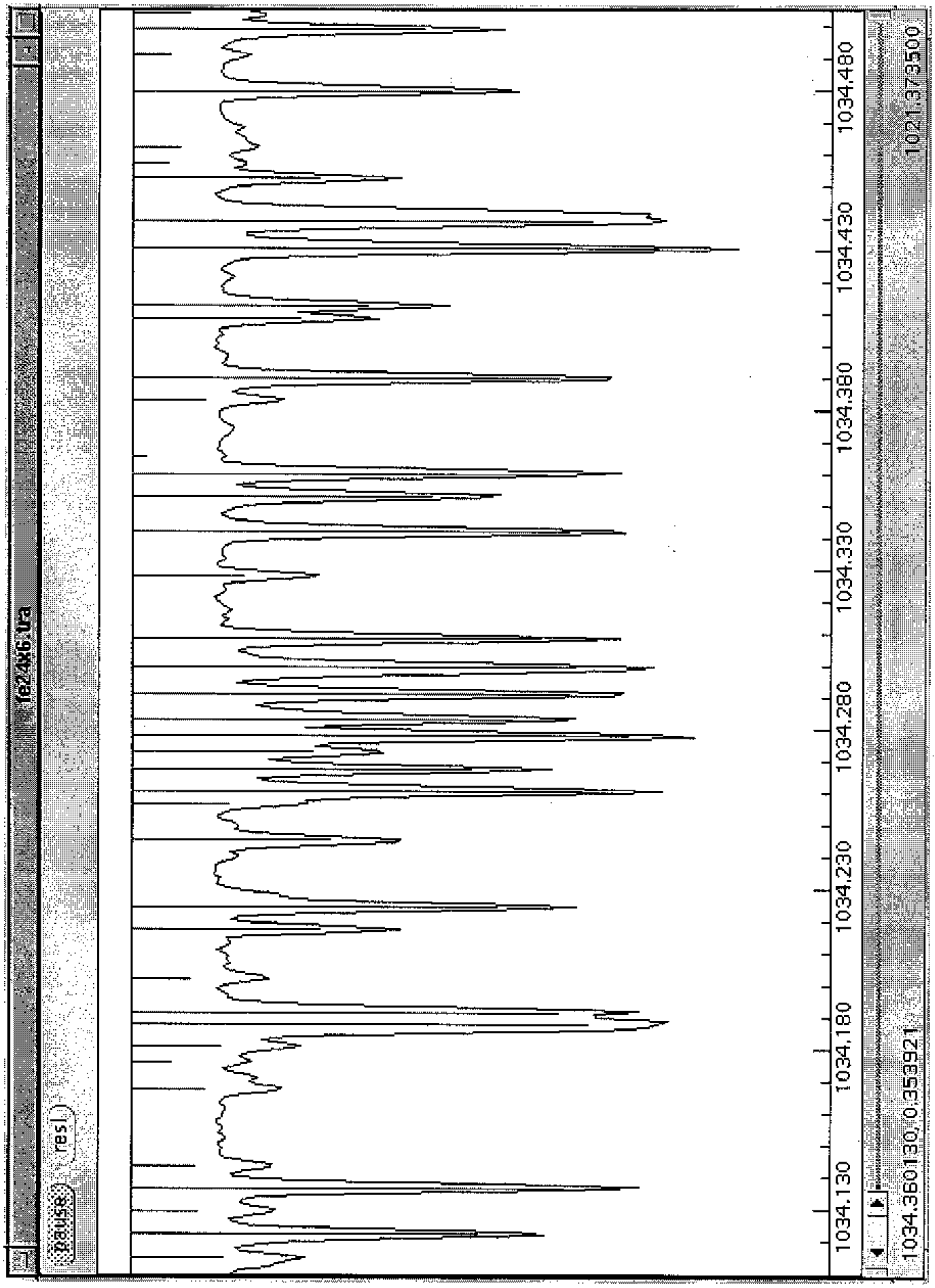
(1x2)E2

```
|                                                    Q_branch
|
|        RP_cal        RP_obs        diff    | J       wv        delta1      delta2      intens   Comm
|  1.                                        |
|  2.    9.098771      9.090890    0.007881  |
|  3.   11.698070     11.697880    0.000190  |
|  4.   14.297104     14.297070    0.000034  |
|  5.   16.895818     16.896050   -0.000232  |
|  6.   19.494151     19.494320   -0.000169  |
|  7.   22.092044     22.091860    0.000184  |
|  8.   24.689440     24.690020   -0.000580  |
|  9.   27.286279     27.286170    0.000109  |
| 10.   29.882501     29.882390    0.000111  |
| 11.   32.478048     32.477960    0.000088  |
| 12.   35.072862     35.072500    0.000362  |
| 13.   37.666881     37.667090   -0.000209  |
| 14.   40.260047     40.259330    0.000717  |
| 15.   42.852299     42.852300   -0.000001  |
| 16.   45.443577     45.443790   -0.000213  |
| 17.   48.033824     48.034050   -0.000226  |
| 18.   50.622977     50.623210   -0.000233  |
| 19.   53.210975     53.211330   -0.000355  |
| 20.   55.797759     55.799490   -0.001731  |
| 21.   58.383269     58.385400   -0.002131  |
| 22.   60.967444     60.971430   -0.003986  |
| 23.   63.550222     63.551350   -0.001128  |
| 24.   66.131542     66.122000    0.009542  |
|                                            |
|                                            |
|                                            |
|                                            |
```

Appendix D

A piece of spectrum of $CH_3^{18}OH$ in the 900-1100 cm^{-1} region captured from the screen.

This is a piece of spectrum captured from the screen during MOSAA running. Three colors appear in this spectrum. Blue lines are normal peaks in the peakfinder file. Red lines represent the peaks already assigned. A green line is the peak currently being searched during the assignment processing.


fe24x6.ua
pause
res
1034.130
1034.180
1034.230
1034.280
1034.330
1034.380
1034.430
1034.480
1034.360130,0.353921
1021.373500

VITA

Candidate's full name :	Jin Wang
Place and date of birth :	Suzhou, Jiangsu, P.R.China October 6, 1971
Address :	262 George Street Fredericton, N.B. Canada, E3B 1J5
Schools attended :	Suzhou No.1 High School Suzhou, Jiangsu, P.R.China 1986-1989
Universities attended :	Suzhou University B.Eng., Computer Science and Application 1989-1993 Suzhou, Jiangsu, P.R.China