Laboratory Spectroscopy of Glycolaldehyde for Interstellar Applications

A Major Qualifying Project Submitted to the Faculty of Worcester Polytechnic Institute in partial fulfillment of the requirements for the Degree in Bachelor of Science In Physics

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Contents

1 Abstract

Interstellar complex organic molecules (COMs) and water are important clues in the search for the origins of life. Distributed throughout the universe in areas with ideal life-forming conditions, like planetary collisions with comets and molecular clouds, these molecules enable and partake in reactions that form major building blocks of life, like RNA.

The importance of these molecules makes them ideal subjects to study. However, the vastness of space and the inability to reproduce interstellar conditions in laboratory settings proposes significant challenges in the collection and analysis of these samples. The development of high-resolution spectrometers mitigates many of these problems, as they collect the desired data through the analysis of the electromagnetic spectrum, which is easily measured from Earth. These devices operate in various parts of the spectrum, including the terahertz region, and allow for the study of molecules' quantum transitions and the extrapolation of relevant information on their structure, composition, and more.

This paper presents the data collection and analysis of the rotational spectra lines of water and glycolaldehyde using Doppler-limited spectroscopy with lock-in detection techniques. These techniques increased the signal-to-noise ratio and amplified the collected signal. This data was collected to enable future spectroscopy studies by providing reference information on the rotational transitions of the molecules.

2 Acknowledgements

We would like to thank everyone who supported us throughout our MQP. The completion of this project and paper would not have been possible otherwise.

We would first like to thank WPI's Laboratory for Education and Application Prototypes (LEAP) Facility for supplying us with the necessary equipment, resources, and workspace.

We would also like to thank our advisor, Professor Douglas Petkie. His continual support and guidance ensured the project was on the right path from the beginning. Every piece of advice he gave was invaluable to both this project and our learning experience. His prior research and work with spectroscopy and glycolaldehyde were crucial to our understanding of the topic and methodology.

We also owe our thanks to Jacob Bouchard for the time he spent in the lab teaching us how to use the equipment and helping us take measurements, along with the invaluable feedback and advice he provided throughout the project. He was crucial in the execution of our vision for this project.

Finally, we thank Kaitlin Mason and Amy Melina Welch for their previous work on this project. The work they put into building the spectrometer and optimizing it allowed us to go straight to the data collection stage of our project with little issue. Kaitlin's detailed report was consistently used in the understanding of the project and the development of our goals. We could not have accomplished what we did without their efforts.

3 Introduction

The origins of the universe and how life began on Earth are still unknown. Hints of these beginnings can be found throughout the cosmos in the interstellar medium (ISM) and in complex organic molecules (COMs), which are identified through gas-phase spectroscopy[1,2,3,4].

The ISM is the blanket of gas, radiation, and dust that makes up the universe[5]. Here, gasses may exist in molecular, ionized, or atomic states and sometimes contain COMs, molecules composed of at least six atoms, one of which is carbon[2,4,6]. The composition and properties of these molecules, along with the contributions of water, result in reactions that form ribose and other important components of RNA and life[7]. Glycolaldehyde (CH_2OHCHO) is a common COM found in the ISM and the biospheres of exoplanets. It is the smallest molecule with both an aldehyde and hydroxyl group, making it an excellent candidate for the formation of life[8,9].

Analysis of these molecules and various spectra in the ISM is impossible to conduct directly due to the vastness of space and the inability to accurately reproduce the interstellar conditions in a laboratory setting. Therefore, spectroscopy is the best way to collect and analyze data by comparing experimental frequencies with those in online databases and published papers[6,10]. For astronomical spectroscopy, the main way to collect data is with a telescope, like the Atacama Large Millimeter Array (ALMA), the Combined Array for Research in Millimeter-wave Astronomy (CARMA), the Atacama Pathfinder Experiment (APEX), the South Pole Telescope (SPT) and SOFIA[11]. These millimeter and submillimeter telescopes are stationed around the world and are actively used by astronomers studying spectra.

The goal of this project was to improve upon the spectrometer that was built during previous Major Qualifying Projects (MQPs) and contribute to the online databases by providing references of glycolaldehyde's spectra.

4 Background

The following sections will explain the terahertz (THz) region of the electromagnetic spectrum (EM), molecules essential for the development of life, like glycolaldehyde and water, and the different types of spectroscopy along with their applications. Details on spectrometers and how they utilize the terahertz region will also be included.

4.1 Terahertz Region of the Electromagnetic Spectrum

The terahertz region of the electromagnetic spectrum lies between the microwave and infrared regions, as seen in Figure 1[12]. The region is generally considered to range between 0.1 and 10 THz, though some consider it to go as high as 30 THz[12,13]. Compared to other regions of the EM spectrum, like visible and microwave, the THz region has historically been underutilized in commercial and scientific applications. As the region's benefits and applications have become more well-known, however, interest in terahertz spectroscopy has expanded greatly[13].

Each region of the EM spectrum is associated with different benefits when utilizing spectroscopy. The visible region is often associated with the electron transitions of single atoms, like hydrogen, whose abundance on Earth and ease of access have allowed their spectra and properties to become well understood[14]. Spectroscopy in the microwave and THz regions of the EM spectrum typically focuses on the lower energy molecular rotations of molecules, which are often associated with the formation of life[13].

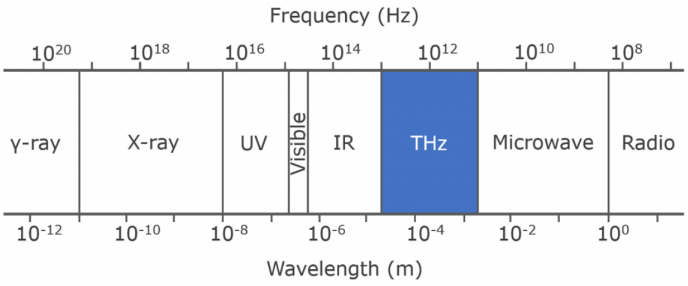


Figure 1: The electromagnetic spectrum[15].

4.1.1 Applications of the Terahertz Region

There are numerous applications of the terahertz region, but this paper focuses exclusively on astronomical applications.

One of the major benefits of utilizing the THz region is that the wavelength, λ, is short enough that terrestrial factors, like atmospheric temperature, pollutants, and water vapor, do not contribute to the noise of spectroscopy data[11,16]. Stations like ALMA are located high in the atmosphere because it allows the radio waves to be detected easier. As the telescopes become closer to sea level, the radio waves have to penetrate through more atmosphere, which in return makes the signal less detectable[16].

The fitted spectral lines to a molecular Hamiltonian are originally found in experimental laboratories, like the one for this MQP, and are then applied to different astronomical bodies like planets, nebulae, and galaxies[11]. The molecular Hamiltonian is an effective model for symmetric and asymmetric top molecules and their resonance interactions. This means the energies of molecules can be described via their rotational transitions[17]. These benefits have created a push to develop and utilize astronomical instruments that can detect wavelengths in the THz region of the EM spectrum[18].

4.2 Molecules Needed for the Development of Life

There are certain elements and molecules that are necessary for the creation of life. Out of the 115 known elements, 19 have been deemed essential for life as they are found in cells, a part of all living organisms, and in RNA and DNA. RNA specifically contains carbon, oxygen, hydrogen, nitrogen, and sulfur. Phosphorus is found in both RNA and DNA[17, 19]. Sugar, a COM, is also needed for the creation of RNA and DNA and is generally composed of some of the 19 essential elements[20].

4.2.1 Water

Water is essential for the formation of life due to its unique ability to behave as a universal solvent and begin the process of forming molecules utilized in the creation of life[21]. Water is plentiful in the ISM and has been detected within molecular clouds, exoplanets, and within the solar system[21]. These factors make water vital to figuring out how life originated in the universe and another important molecule to detect and analyze through gas-phase spectroscopy.

Water's abundance in locations where life may form is particularly important. If the molecular building blocks of life are present on an interstellar body, they need to be able to react with each other and form COMs and other vital materials for life, like RNA and DNA. Many of these chemical reactions can only happen if a solvent breaks down the interacting molecules, allowing them to move and react with each other to form a new molecule[21]. Water is able to dissolve more molecules than most other liquids, making it a universal solvent[22].

The locations of water in the ISM can be detected and analyzed with THz spectroscopy. Water is particularly well suited to this kind of data collection as it is a light molecule with a weight of only 18 amu, which results in a sparse rotational spectrum compared to other heavier molecules[23,24]. Studies have been done with water in the 200 GHz to 2400 GHz range as well as at 183.310 GHz specifically, as this is a pure rotational transition of the molecule[25,26].

4.2.2 Complex Organic Molecules

Every atom originated in the early universe, shortly after the big bang. Over time, these atoms have condensed into elements, forming everything that makes up the ISM, including stars. As these stars die, they expand and explode, filling the surrounding areas with the elements once contained inside them. New stars are eventually fused, restarting the cycle of life and leaving all of the dispersed elements other than hydrogen in the ISM. These remaining elements lead to the formation of planets, moons, asteroids, and sometimes complex molecules. This process is visualized in Figure 2. If these complex molecules contain carbon, they are classified as complex organic molecules, since carbon is one of the 19 essential elements for life[2,4].

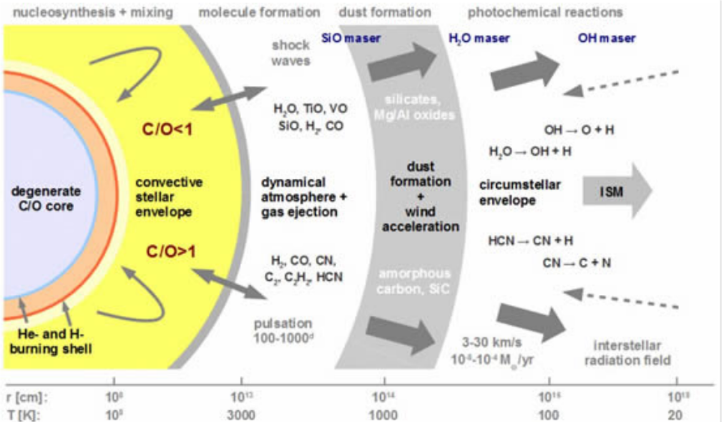


Figure 2: Visual representation of the death of stars and the resulting formation of molecules[27].

4.2.3 Glycolaldehyde

Glycolaldehyde (CH_2OHCHO), depicted in Figure 21, is one of the simplest COMs and has been detected in numerous locations throughout the ISM, including comets and near the Sagittarius B2 molecular cloud complex[8,10]. As a simple sugar, glycolaldehyde can react with propanol to form ribose, an essential component of RNA[9]. Its abundance and abilities mean glycolaldehyde could help unlock the secrets of life's origins, which makes it an important molecule to detect and analyze through gas-phase spectroscopy.

The distribution of glycolaldehyde throughout the ISM gives rise to many exciting possibilities and theories. One of the major theories for the origin of life is the panspermia theory, which argues that life began on Earth after essential life-building molecules, like glycolaldehyde, were deposited on the planet by comets[29]. Experiments conducted at NASA's Johnson Space Center have determined that it is possible for glycolaldehyde to survive a comet's impact with Earth, which adds validity to both the panspermia theory and the possibility of glycolaldehyde having a vital role in the origin of life[8].

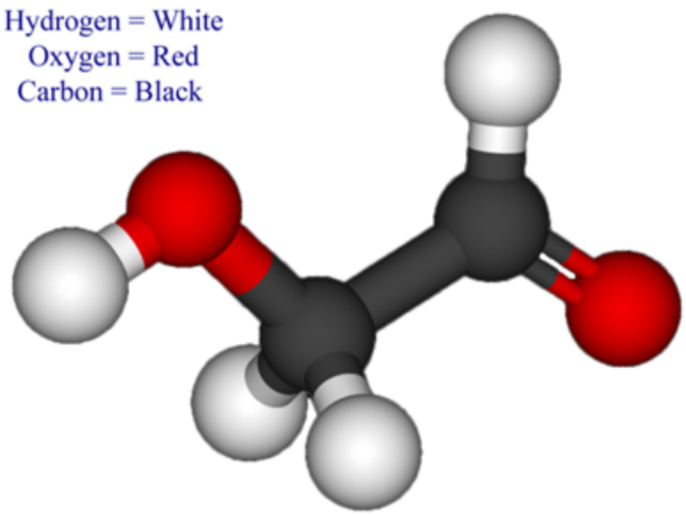


Figure 3: The molecular structure of glycolaldehyde, which contains a double bond of carbon and oxygen[28].

Glycolaldehyde has also been detected near Sagittarius B2, a molecular cloud of gas and dust[10]. It is predicted that the conditions of molecular clouds like this allow for the formation of COMs, which could explain both glycolaldehyde's origin in the ISM and how it gets onto the comets essential to the panspermia theory[9,30].

None of these theories have been proven or disproven, and the origins of life in the universe are still shrouded in mystery, making the detection and study of glycolaldehyde and other COMs vital to many scientific fields. These studies are frequently done with THz spectroscopy and have made use of glycolaldehyde's millimeter and submillimeter spectra between 13.48–22.14 GHz, 72–122.5 GHz, and 128–354 GHz[10,31]. Portions of the ranges, like 13.48–22.4 GHz and 71–103 GHz, have been detected in the ISM with the Green Bank Telescope (GBT) and the National Radio Astronomy Observatory (NRAO) while other portions are predicted values from laboratory studies[31]. Regardless, glycolaldehyde's unique absorption lines are visible at these frequencies, allowing it to be detected within the spectra of the ISM and studied in laboratory settings.

4.3 Spectroscopy

Spectroscopy is the study of a molecule's absorption and emission of electromagnetic radiation following a change in energy state. This change is caused by specific interactions within the molecule on the quantum level and results in the molecule absorbing electromagnetic radiation which creates unique spectrum, as seen in Figure 4. The uniqueness of the spectrum makes it an easy and accurate way to identify a specific molecule's presence within an interstellar body, like a nebula or star[14]. These spectra can also provide important information about the molecule, like their rotational and vibrational spectral transitions, elemental composition, temperature, and density[13,32].

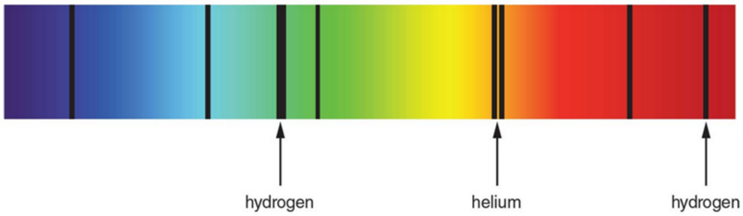


Figure 4: The absorption spectra of hydrogen and helium. These spectra are created after a hydrogen or helium electron is excited and changes energy states, resulting in the absorption of certain wavelengths, which creates the black lines in this diagram[33].

The different types of quantum interactions result in three types of spectroscopy. The frequent utilization of these across many different fields of study has resulted in numerous sub-categories of spectroscopy, including terahertz molecular absorption spectroscopy[34]. Studying interstellar molecules is of great importance, though it can be incredibly difficult to do as collecting samples from space and replicating interstellar conditions in a laboratory is almost always impossible[32]. Spectroscopy, in general, removes these difficulties as it utilizes electromagnetic radiation which can be studied regardless of distance. Terahertz spectroscopy further removes difficulties with data collection and analysis as the shorter wavelengths found in the terahertz region have higher angular resolutions than other wavelengths, like microwaves[35].

These benefits of spectroscopy in general and terahertz spectroscopy specifically have made this form of spectroscopy very popular in recent years. Heterodyne instruments have been launched into space to collect spectra up to 600 GHz and there are numerous telescope and satellite arrays stationed on Earth, like ALMA, CARMA, APEX, SPT, and SOFIA, which collect spectra from various ranges in the THz region of the EM spectrum[11]. The data collected from these instruments result in spectra as seen in Figure 5.

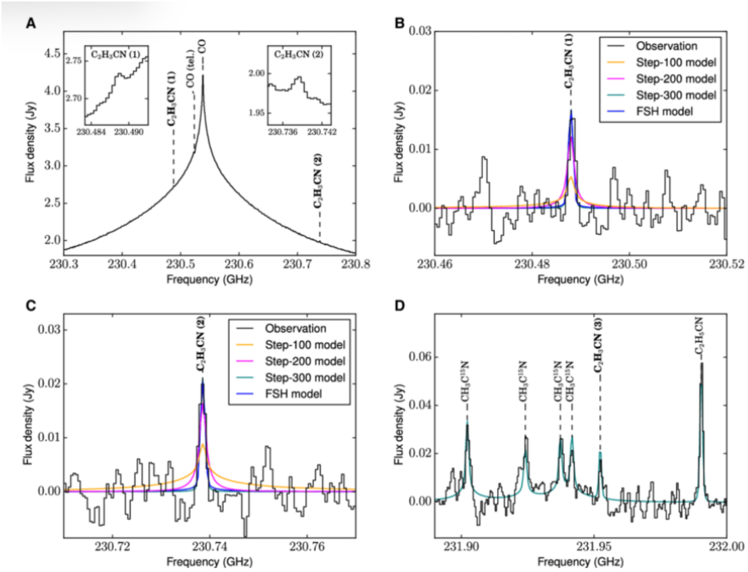


Figure 5: The spectra of three of C_2H_3CN's transitions based on data collected by ALMA[36].

The specific spectrometer setup for this project involved high-resolution rotational spectroscopy and an absorption spectrometer that used a frequency-modulating lock-in detector.

4.3.1 Molecular Spectroscopy

Molecular spectroscopy measures the radiation absorbed or emitted by a molecule following a change in its vibrational or rotational energy states[34,37]. These changes abide by the photon-energy relationship, which is detailed in Equation 1:

$$E_{high} - E_{low} = h\nu \tag{1}$$

where E_{high} represents the higher energy state, E_{low} represents the lower energy state, h is Planck's constant, and ν is the frequency of the absorbed or emitted radiations[34]. The resulting frequency creates characteristic spectra which provide information on the qualities of a molecule's structure as well as its environment, like temperature and pressure[38].

The generated spectra are dependent on unique characteristics, like molecular structure, moments of inertia, and the specific change in energy that occurred[38]. The rotational energy level structure of a molecule is visualized in Figure 6 and shows that the structure creates equally spaced rotational frequency transitions with a spacing of $\nu = \frac{2B}{h}$, where B is the molecular constant and is detailed in Equation 2[39]:

$$B = \frac{h}{8\pi^2 I} \tag{2}$$

where h is Planck's constant and I is the inertia, which is directly proportional to mass[40]. These relationships mean the spacing and change in energy levels are inversely proportional to the mass of a molecule, resulting in low energy transitions of heavier COMs, like glycoaldehyde.

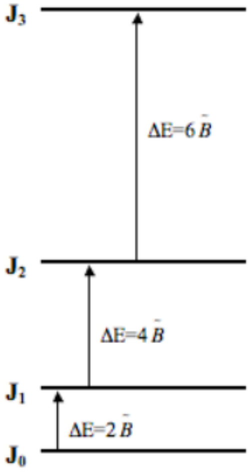


Figure 6: Example of changes in energy levels[23].

As equation 1 details, the energy is directly proportional to the emitted frequency, which in turn is inversely related to the generated wavelength. The low energy transitions of complex organic molecules result in larger wavelengths, like those found in the THz region of the EM spectrum.

The size of the wavelengths of these molecules has no effect on molecular spectroscopy, as it can be conducted in any region of the EM spectrum, though it traditionally makes use of spectra found in the infrared region, which often overlaps with vibrational spectroscopy, as seen in Figure 7. Spectra in the THz region are often avoided as most molecules' vibrational quantum numbers fall outside the THz region, so it is easier to simply study the molecular spectra of smaller atoms[38,41].

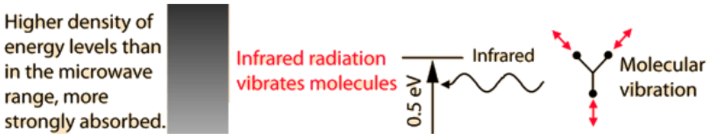


Figure 7: This is the vibrational spectroscopy in the infrared region of the EM spectrum[42].

4.3.2 Absorption Spectroscopy

Absorption spectroscopy analyzes the absorption spectrum of a molecule. This form of spectroscopy can be done in any region of the EM spectrum, though it frequently utilizes the terahertz region of the electromagnetic spectrum as low-energy large-wavelength photons have the ability to change a molecule's rotational state to create unique absorption spectra and peaks. The specific wavelength is unique to the molecule as it depends on characteristics such as atomic weight, structure, chemical bond strength, and interactions between the molecule and its environments[43,44].

The wavelength that an absorption peak and spectra occur at is determined by both the observed molecule and the Beer-Lambert law, shown in Equation 3:

$$A = log\frac{I_0}{I} = lc\epsilon \tag{3}$$

where A is the absorbance, I_0 is the incident intensity, I is the transmitted intensity, ϵ is the molar absorption coefficient, l is the length of the light path, and c is the concentration of the molecule[44,45,46]. An absorbance of zero indicates that no excitation occurred while the magnitude of the molar absorption coefficient is directly proportional to the probability of changing rotational energy levels[46].

4.3.3 Rotational Spectroscopy

The majority of gas-phase molecules in the ISM have been discovered through rotational spectroscopy[1]. Similar to other types of spectroscopy, each molecule has its own unique rotational signature, which led to the initial discovery of the presence of these molecules, like glycolaldehyde, in the ISM[10,32]. In order to look at the rotational transitions, the vibrational transitions also need to be known, as seen in Figure 8. Rotational spectroscopy involves exciting a molecule with a photon resulting in an energy transition between rotational levels in a molecule. This transition reveals information on the molecule's geometry, which includes its bond lengths and distribution of atomic mass, as described by moments of inertia. This is especially prominent in asymmetric molecules, like glycolaldehyde, as seen in Figure 9, which shows that the rotational states need less energy for transitions than the vibrational states do[48]. This is especially useful when looking at molecules at extremely low pressures and temperatures, like those found in the ISM[47].

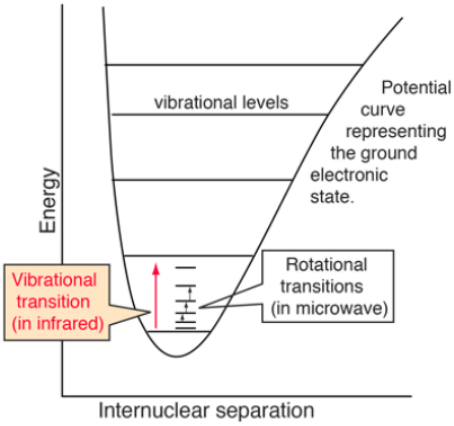


Figure 8: This is a large-scale depiction of a molecule's vibration and rotational transitions. Note the scale difference between the two types of transitions, allowing for observations in their respective parts of the EM spectrum[47].

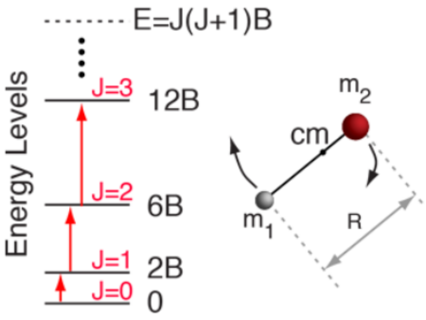


Figure 9: This shows how the rotation of the molecule affects the energy level, where J is the rotational angular momentum[47]. While this depicts a diatomic molecule, the concept also applies to complex molecules.

4.4 Spectrometer

In general, spectral data is obtained through the use of a spectrometer, which analyzes variations of specific physical characteristics within a predetermined range[49]. The spectrometer typically contains a holding cell for the sample, a dial to control how much sample is allowed into the measuring area, and a sensor and detector on each side of the cell to take the desired measurements. The detector is often connected to a computer or oscilloscope to digitize the measurement, which the user then interprets[50]. The produced measurements can contain three types of spectra: continuous spectra, emission spectra, and absorption spectra, all shown in Figure 10. Continuous spectra contain no breaks or dips in the data, while emission spectra exclusively contain the peaks. Absorption spectra are considered continuous spectra minus emission spectra, which is the type of spectroscopy in this project[51].

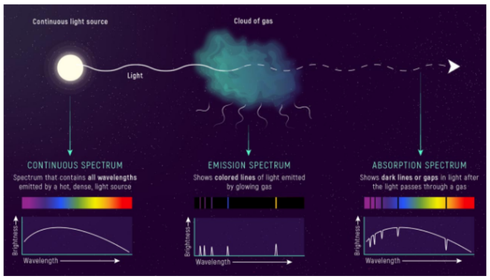


Figure 10: Examples of the different spectra data from a spectrometer.

5 Methodology

This section details the properties of the spectrometer and the data collection process.

5.1 The Set Up

The spectrometer is composed of three interconnected systems as seen in Figure 11. The systems include the source, the absorption cell, the vacuum system, and the sample, along with the noise reduction and the signal conditioning amplifiers.

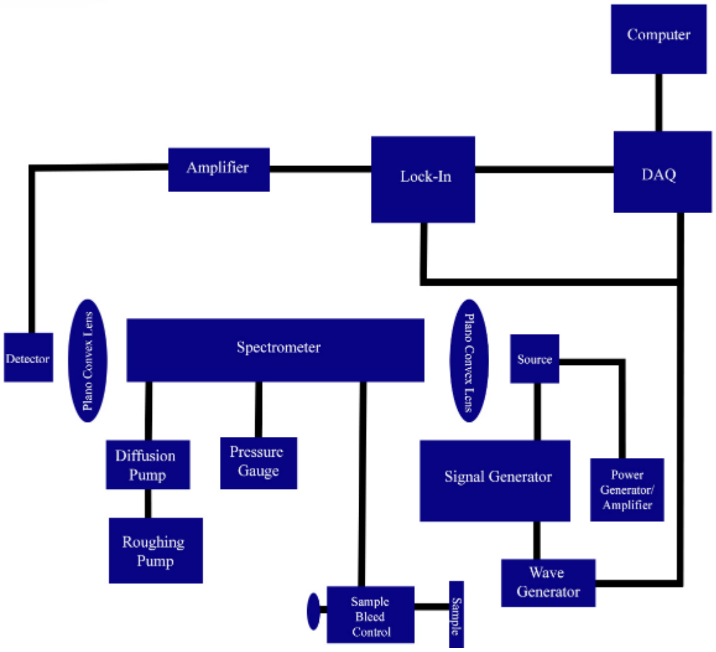


Figure 11: This is the block diagram of the full system.

5.1.1 The Source

The first part of the system is the output and the references. Figures 11 and 12 show that the output of a signal generator is connected to the power supply/multiplier, which generates electromagnetic radiation allowing the observer to collect data. The power supply/multiplier is a six times multiplier, so the generated frequency is six times what the user inputs from the signal generator. The spectrometer typically operates in the 140-220 GHz frequency region with output powers of approximately 1 mW and is driven by the signal generator in the 23-36 GHz range.

The source is also connected to the signal and wave generators, which allows for two forms of frequency modulation. The primary modulation is a ramp function produced by the signal generator, which is set to the middle frequency of the sweep. For water this frequency was 183.310 GHz and for glycolaldehyde, it was 183.416 GHz. The ramp function is set to the amplitude of 20 MHz, which is half of the span length of 40 MHz. Each sweep is completed at a rate of 1 Hz. The secondary modulation is the sine wave produced by the wave generator at a frequency of 20.0 kHz with a reference amplitude of 500 mV, which is then translated into the same frequency amplitude.

Figure 12: The output and reference part of the spectrometer. Circled from top left to bottom right: the wave generator, the power supply/multiplier, the signal generator, and the output.

5.1.2 The Absorption Cell

The terahertz radiation sent through the system is collimated by a plano-convex lens, which is a certain distance away from both the cell and the output source in order to maximize the power traveling through the cell. The cell itself is a two-meter acrylic tube that is completely sealed off from the lab and is pictured in Figure 13. In the middle of the cell is a pressure gauge, which allows us to make sure the system is at space-like conditions and lets us know how much sample is in the cell as an increase in pressure indicates an increase of sample.

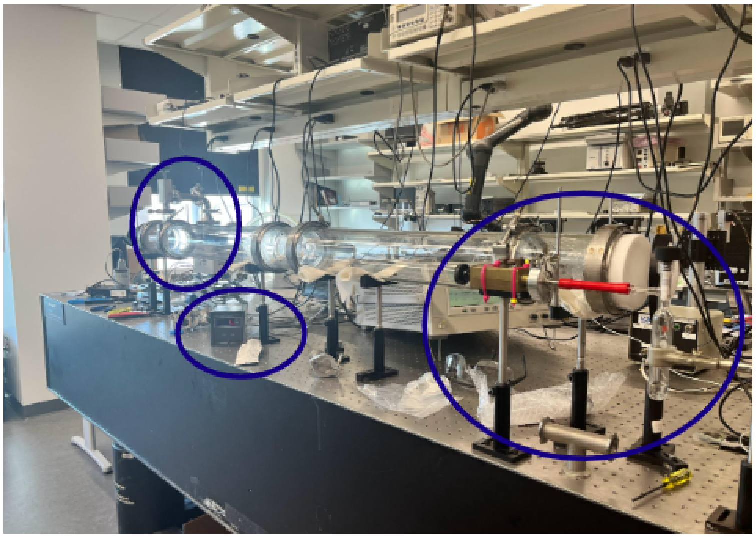


Figure 13: The cell of the spectrometer with the three subsections, seen in blue circles. From left to right, are the diffusion pump, the pressure gauge, and the sample.

5.1.3 The Sample

From left to right in Figure 13 are the diffusion pump, the pressure gauge, and the sample. The sample is located closest to the output and is attached to the bleeder, which allows the user to control how much of the sample is allowed into the cell. Next to it is the pressure gauge, which displays the pressure of the cell in mTorr or Torr.

5.1.4 The Vacuum System

On the opposite end of the cell from the sample is the vacuum pump seal, which is connected to two different pumps. The larger pump is the roughing pump, which is pictured in Figure 14. This pumps the system down from atmospheric pressure, about 760 Torr, to approximately 20 mTorr. The diffusion pump is the smallest of the two pumps and pumps out the rest of the air in the cell to mimic space-like conditions by keeping the cell well below 1 mTorr, which is considered a vacuum with no sample remaining. The sample bleeder and vacuum valves can be adjusted to allow a sample pressure of approximately 10 mTorr which is the typical operating pressure where the line widths are still within the Doppler-limit. Under these conditions, decreased frequency resolution due to pressure broadening, which occurs at higher pressures, is avoided.

Figure 14: The roughing pump.

5.1.5 The Noise Reduction and Signal Conditioning Amplifiers

The final section of the spectrometer is the noise reduction and the amplifier. Here, the terahertz power leaves the cell and passes through another plano-convex lens resulting in the focusing of the signal onto the detector, as seen in Figure 15.

From the detector, the signal goes through a low-noise pre-amplifier, shown in Figure 16. This reduces the noise in the signal, allowing the signal and data to be read more clearly. When the frequency is modulated, the low-pass and high-pass filters are set to pass the modulation frequency, typically at 20 kHz. For a more detailed list of the settings see Table 1.

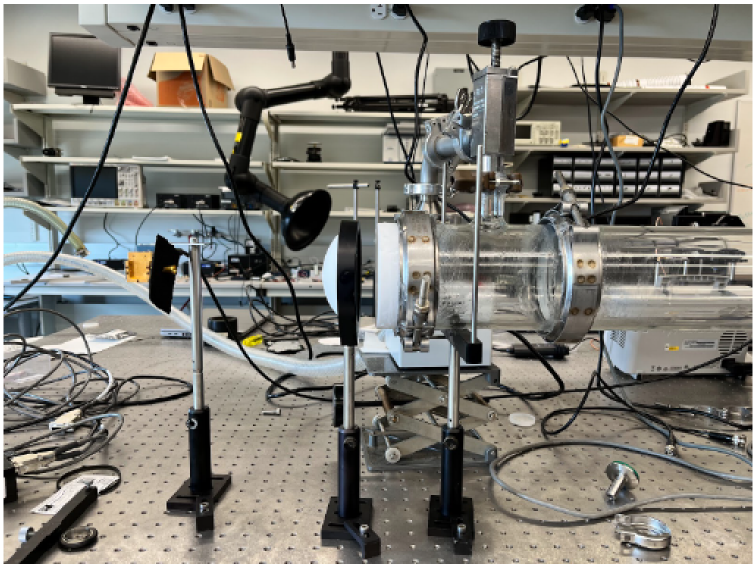


Figure 15: The detector end of the spectrometer.

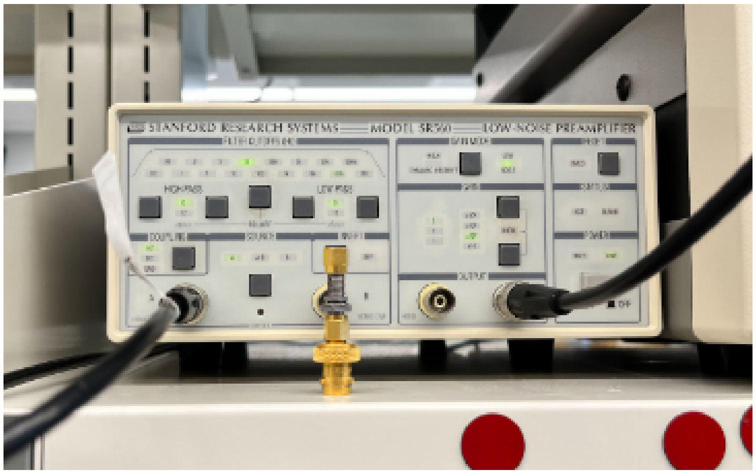


Figure 16: The pre-amplifier that minimizes the noise to produce a cleaner signal.

After this, the cleaner signal passes through the lock-in, as seen in Figure 17 and the exact settings are found in table 1. The lock-in uses the reference from the wave generator and maps it onto the detected signal. The output is then digitized via the DAQ assistant. The DAQ has two functions the first is to collect a certain number of samples in one second, we had this set to 10,000 samples per second and collected data for 3 seconds to ensure a full sweep was collected. The other function receives the ramp function from the signal generator, allowing the user to better recognize the start and the end of each sweep taken.

preamp	low filter cut off	30 Hz
	high filter cut off	100k Hz
	low roll-off intensity	6 dB
	high roll-off intensity	6 dB
	gain mode	low noise
	gain	$5 * 10^2$
lock-in	time constant	1 ms
	sensitivity	1 V
	input range	1 V
	reference wave	sine wave
	filter	6 dB

Table 1: This table includes the setting of the low-noise amplifier and the lock-in.

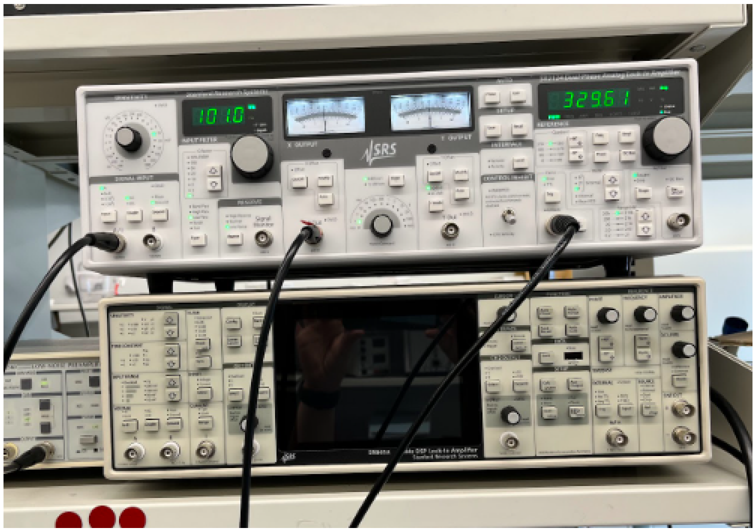


Figure 17: The lock-in amplifier. It maps the reference wave from the wave generator to the detected signal.

5.2 Turning On the System

In this section, we assume the entire system has been turned off, including the roughing and diffusion pumps, as well as all of the electronics. We will then go through the steps required to turn on the entire system and collect high-resolution spectra.

The first step to setting up the system for data collection is to prepare the sample gas handling and vacuuming system for the absorption cell. The sample gas inlet valves should be closed off from the sample holder to the absorption cell and samples of either water or glycolaldehyde can then be placed in the sample holder while the system is off. Doing this while the cell is closed and the system is off prevents the pressure inside the cell from skyrocketing and damaging the pumps and other components. The diffusion pump can only operate at pressures below 100 mTorr and higher pressures can cause the oil in the diffusion pump to burn and backfill into the absorption cell.

After the sample is inserted and the absorption cell is sealed off from the outside environment, the system can be turned on. The process of turning it on must be done in a specific order to prevent the components from becoming damaged and the system from catastrophically failing. First, the cell is opened while the sample and sample bleeder are closed off. The roughing pump is then turned on, allowing the system to eventually come to a constant pressure of around 50 mTorr, which can take several minutes.

When the pressure gauge indicates the cell is at constant pressure below 100 mTorr, the sample remains closed off and the diffusion pump is turned on. The pump takes approximately 15 minutes to warm up, and during this time the pressure may go up by several 10s of mTorr. After the diffusion pump is warmed up, the pressure will drop to below 1 mTorr, and the cell is now considered to be under a high vacuum.

To prepare the sample, the air in the headspace of the sample needs to be removed. For this to happen, the bleeder valve is repeatedly opened very slightly and closed in a 'pulsing' manner. This allows the pressure to jump to over 100 mTorr and go back down, which eventually allows the vapor pressure of the sample to fill the sample container's headspace. Despite the pressure jumping to high values over 100 mTorr, even higher pressures, like those above 500 mTorr, should be avoided to prevent damage from occurring to the system.

At this point, one of two approaches can be taken to fill the absorption cell with the sample gas and bring the pressure to about 10-20 mTorr. The first option is to close off the diffusion pump and isolate the cell. The bleeder valve is then slightly pulsed open to fill the cell to the target pressure.

If the pressure slowly rises from the cell outgassing, then the second approach must be taken. Both the diffusion pump valve and bleeder valve must be slowly opened to create a slow and constant low-pressure flow of the sample at the target pressure of around 10-20 mTorr

Once either of these steps has been completed, the spectra can be recorded near the Doppler-limit. If the pressure in the cell drops, the line strength will start to decrease. If the pressure increases, the line may grow a bit stronger, but eventually, only the linewidth will increase due to pressure broadening.

Now, the THz source, detector, and signal conditioning electronics can be turned on in a specific order. First, the power supply to the VDI frequency multiplier-chain is turned on, followed by the SRS detector pre-amplifier, the lock-in amplifier, the wave generator, and the Agilent signal generator, which drives the frequency multiplier chain.

5.3 Collecting Data

To collect the desired data, the sample and sample bleeder were opened, as described above, allowing the molecule sample to flow into the cell. When the flow resulted in constant pressure on the pressure gauge, a LabVIEW virtual instrument (VI) was run. The VI digitized both the linear frequency ramp generated by the signal generator to sweep the frequency and the signal from the lock-in amplifier. The VI also collected a specific number of voltage samples at a specified rate and time interval, which was determined by the settings on the DAQ. The VI then generated a graph of these voltages, which presented a visualization of the molecule's absorption spectra. This data was later exported to Igor Pro 9 for further analysis. The code for the LabVIEW VI can be found here.

5.4 Turning Off the System

Similar to turning on the system, there is a specific order for turning everything off so the system does not catastrophically fail. The system must also be at low pressure, as turning off the components while there is high pressure in the cell will cause damage.

If the pressure is adequate, the sample and sample bleeder are closed off from the cell, though the cell itself remains open while the diffusion pump is turned off, as this allows the diffusion pump to cool down while the roughing pump remains on. The diffusion pump has a fan and light indicator that remain on until it is cooled down, at which point these automatically turn off. Once the diffusion pump has cooled, the roughing pump can be turned off. The cell pressure will slowly come back to near atmospheric levels and the cell can be closed off.

While waiting for the diffusion pump to cool down, most of the other components can be shut off. The wave/function generator is turned off, followed by the Agilent signal generator, pre-amplifier, and lock-in. After running through a visual check that those components are off, the power supply/multiplier is shut off. By this time, the diffusion pump usually shuts off and the roughing pump can be turned off.

If the sample in use is water, the sample and sample holder may be left attached to the system, as water retains its state and desired properties at room temperature. If the sample is glycolaldehyde, the sample must be removed and stored properly as glycolaldehyde melts at room temperature. However, this can only be done when the system is off and the sample is sealed off from the cell to prevent the cell's pressure from skyrocketing and components from becoming damaged.

6 Analysis

In this section, we look at how to analyze the collected data using Igor Pro 9 and its multipeak analysis tool as well as a code that simulates this process. For both water and glycolaldehyde, the collected data were differentiated and smoothed multiple times which allowed us to see exactly where the peaks were. The peaks should appear at the known or predicted values for the molecule's rotational transitions.

6.1 Water

We collected the direct absorption of water to make sure the system was running properly. As mentioned previously, there is a known rotational transition of water at 183.310 GHz. Water is a small asymmetric rotor with 18 amu that results in a very spare, but strong, spectrum in the THz region. This specific rotational transition was chosen due to it being within the parameters of the spectrometer. The collected data, seen in Figure 18, gave us a general location for the peak.

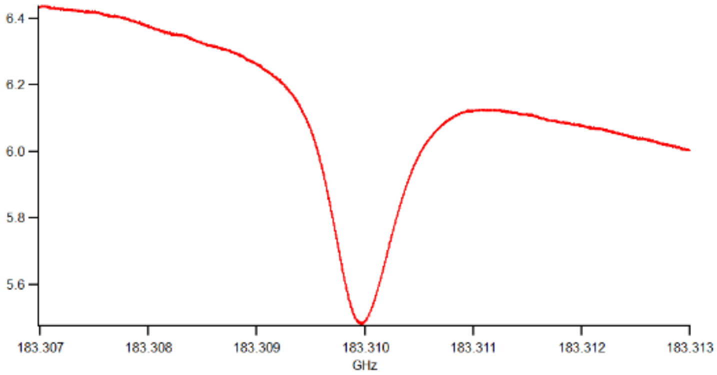


Figure 18: The collected data from the sample of water at 70 mTorr. The x-axis is in GHz since this will allow for more accuracy when analyzing the peak. The y-axis is in volts, allowing us to see the drop in voltage at the rotational transition. The units of the axes are the same for Figures 18 through 23.

After the data is collected, it is differentiated and smoothed twice to clearly see the peak, as seen in Figure 19. This process is done twice to highlight where there is and is not signal, which results in a second derivative lineshape from the absorption spectrum. This allows the peak to easily be identified and for any slowly varying baseline effects due to power variations to be removed.

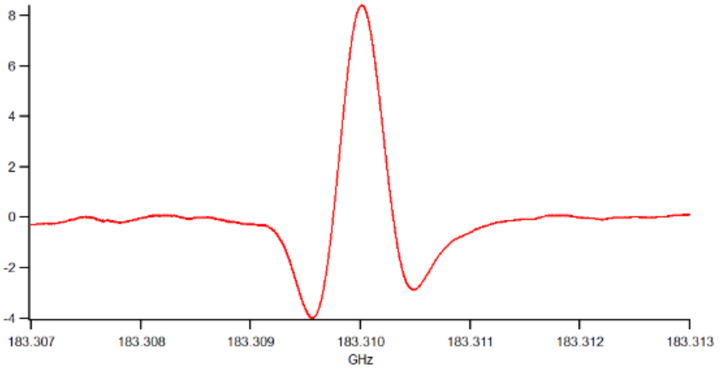
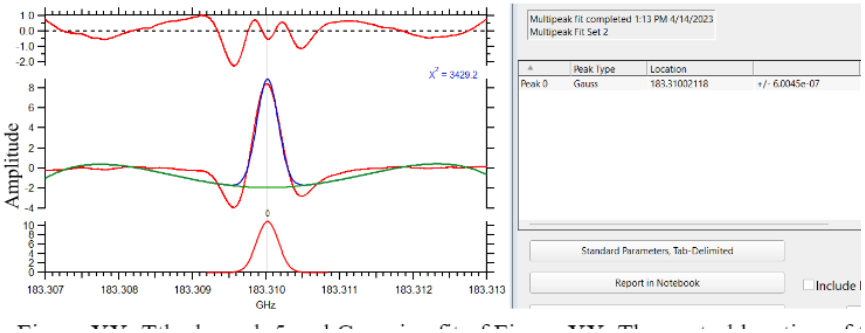


Figure 19: Twice differentiated and smoothed graph of the collected data from Figure 18.

As pictured in Figures 18 and 19, it is evident that the peak is at 183310 MHz, as predicted. We still used a multipeak setting in order to get an even more accurate value, as seen in Figure 20. The multipeak package allowed us to see the exact location and amplitude of the central peak for the water sample. To get the most accurate fit with this package, we use the logpoly5 fit for the baseline as well as the Gaussian fit. The logpoly5 fit was used because it most accurately represents the data and the other baseline fits do not have enough terms to fully describe the curve.

For the specific fit, there are three options: Gaussian, Lorentzian, and Voigt. Gaussian is the fit of a Gaussian distribution, which is usually best for pressures below 200 mTorr. The Lorentzian fit is narrower and better suited for pressures closer to 1 Torr. The Voigt fit is the combination of the two and is suited for pressures between 200 mTorr and 1 Torr. Since we kept our pressure below 200 mTorr, the Gaussian fit was the most logical to use.

As seen in Figure 20, we saw that the experimental value of water was extremely accurate to the known value of 183310.022 MHz. This made us confident that the system was working properly and that we could accurately measure glycolaldehyde.



Multipeak fit completed 1:13 PM 4/14/2023
Multipeak Fit Set 2

	Peak Type	Location	
Peak 0	Gauss	183.31002118	+/- 6.0045e-07

Figure 20: The logpoly5 and Gaussian fit of Figure 18. The central location of the peak is 183310.022 ± 0.001 MHz.

6.2 Glycolaldehyde

The analysis process for glycolaldehyde was almost the same as what we did for water. The collected data is shown in Figure 21, note that this is the first derivative because the direct absorption data was not visible enough. The main difference between water and glycolaldehyde is that there are two peaks that are caused by a doublet, or two rotational transitions within close proximity to each other. This doublet's rotational transition was one of the stronger transitions predicted and located near the transition frequency of water, all while being within the frequency range of our system. Therefore, this doublet was the targeted transition of glycolaldehyde as it was predicted to be feasible by the spectral analysis[10].

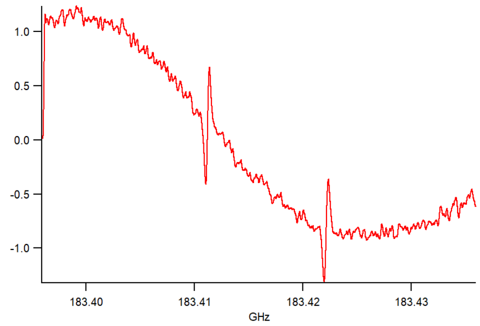


Figure 21: The smoothed collected data of the Glycolaldehyde at 18 mTorr. The x-axis is in GHz due to a larger sweep and the y-axis is still in volts. This graph shows the collected first derivative spectrum captured using a lock-in amplification technique.

After completing the data analysis process explained in the previous section, we are left with Figure 22. Similar to the process for water, this data can then be fit in order to find

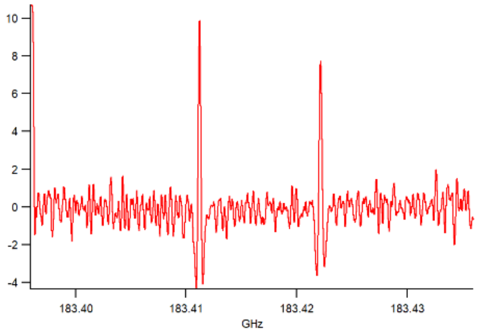
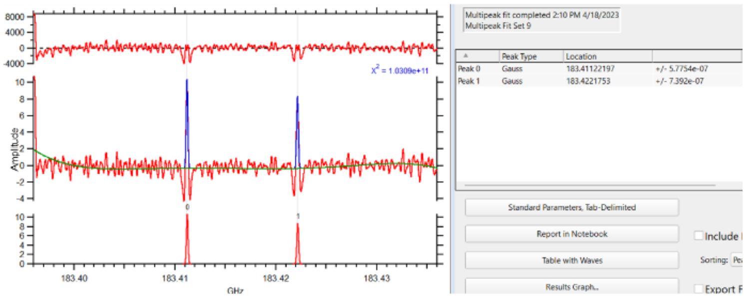


Figure 22: The differentiated and smooth version of the data from Figure 21.

the exact location of the peak, as seen in Figure 23.



Multipeak fit completed 2:10 PM 4/18/2023
Multipeak Fit Set 9

	Peak Type	Location	
Peak 0	Gauss	183.41122197	+/- 5.7754e-07
Peak 1	Gauss	183.4221753	+/- 7.392e-07

Figure 23: The fitted version of Figure 19. The location of peak 0 is 183411.2220 ± 0.0006 MHz and peak 1 is at 183422.1753 ± 0.0007 MHz.

6.3 Simulation

In addition to the collected data, we used Python to code a simulation of the data collection and analysis processes. The simulation allows the user to modify the central frequency, amplitude, pressure, modulation steps, modulation frequency, and modulation amplitude. The ranges of the variables are based on the constraints of the spectrometer that was used in this MQP. The simulation can also be run with either random or specific values that the user chooses and can be found here. Due to time constraints, the amplitude modulation was never completed. This part of the code would allow the user to manipulate how large the amplitude of the sine wave is for each step.

7 Discussion

Comparing the collected data to the predicted data, we can see that the predicted values for these rotational transition peaks are within the uncertainty. From Figure 23, we can see that the measured values are at 183411.2220 ± 0.0006 MHz and 183422.1753 ± 0.0007 MHz. As previously discussed, the study by Weaver, Butler, Druin, Petkie, Dyl, De Lucia, and Blake states that the predicted values for this doublet should be around 183411.066 MHz and 183422.205 MHz[10]. Using a basic error analysis, we can see that the first transitional state has an $8.14 * 10^{-5}$ percent error and the second has $1.4 * 10^{-5}$ percent error.

While the fitted lines in Figure 23 report an uncertainty of a fraction of a kHz, it is common to report an uncertainty of approximately 10-50 kHz to account for any frequency-dependent variations of the system and reproducibility of identifying the peak of a spectral linewidth on the order of approximately 1 MHz. Therefore, the measured lines are in excellent agreement with those predicted by the previously mentioned study.

The comparison of the predicted intensities between the 183 GHz water transitions and the glycolaldehyde doublet is not as favorable. It is expected that the glycolaldehyde doublet would have a similar line strength with about 30% absorption in the system. However, the direct absorption spectrum was difficult to observe as it had a low signal-to-noise ratio. We switched from direct absorption to utilizing frequency modulation and the lock-in to capture the first derivative spectrum shown in Figure 23. This is likely due to water being part of the glycolaldehyde sample, which caused a fractionation between the two gas samples.

The vapor pressure of water is 17.5 Torr and the vapor pressure of solid glycolaldehyde is 4.97 Torr, allowing a significant level of water into the absorption cell. A drying agent or vacuum distillation are approaches to removing water from the glycolaldehyde sample and we could verify this assumption by monitoring the relative intensities of the water and glycolaldehyde transitions to determine the relative concentration of each gas.

8 Recommendations for Future Work

There are a lot of different topics this project could focus on in the future, but it would be most beneficial for future projects to begin with some maintenance to the cell before running measurements. There is a small leak in the cell, which does not pose a safety risk and is small enough at 15 mTorr per minute to not negatively affect the collected data. It is still not ideal to have the leak remain, as it does prevent small amounts of sample from being bled into the cell and measured. The leak in the cell should be fixed and it should also be vacuum distilled to remove traces of previously measured molecules, as mentioned earlier.

Once these are completed and the system is optimized for future measurements, glycolaldehyde can be further studied. As discussed earlier, glycolaldehyde's ranges include other frequencies that the system can detect, and these could be studied the same way as the doublet this project analyzed. Some of the settings on the system's components could also be modified, allowing future projects to not only study a rotational transition of glycolaldehyde but also see how the system's specific settings affect these measurements.

There are also other rotational transition frequencies of glycolaldehyde that can be studied if the system is modified to allow for their detection. This modification would involve finding a new signal generator that would interact with the rest of the system to allow for the detection of frequencies outside of the current signal generator's range. After the signal generator is changed and there is confirmation that the system has been modified properly, settings on other components of the system could be changed while studying these frequencies to again see how the system's specific settings affect the measurements.

Future projects could also shift their focus away from glycolaldehyde and onto other interstellar molecules that are potentially involved in the creation of life and can be measured using the spectrometer. Over 200 total molecules have been identified in the ISM, though not all of these are complex organic molecules or easy to measure with the current spectrometer setup[52].

C_3H_4O, also known as both propenal and acrolein, can react with glycolaldehyde to form ribose, making it an important interstellar COM to study[53]. It is ideal to work with using the current laboratory setup as it is a liquid at room temperature and safe to work with if the handlers abide by standard laboratory safety practices and those specific to acrolein, which can be found extensively online[54,55].

Acrolein's electronic and vibrational spectrum occur between 993 cm^{-1} and 3097 cm^{-1} as well as between 25851 cm^{-1} and 30071 cm^{-1} and these frequencies could provide a basis for the study of the pure rotational spectrum of 8 to 180 GHz in various vibrational states[56,57,58]. A future project could look into replacing the current signal generator with one whose capabilities allow acrolein's transitions to be observed over a broader frequency range. The system could also be kept as is and the pure rotational spectrum could be studied without the basis provided by the electronic and vibrational spectrums.

Dimethyl ether, C_2H_6O, has been detected in both planet-forming discs and star-forming regions[59]. It is one of the most abundant interstellar complex molecules and is capable of reacting with carbon monoxide and water to form acetic acid, another interstellar COM that is used during metabolic processes and produced by some bacteria[60,53,61]. Dimethyl ether is a gas at room temperature while acetic acid is a corrosive liquid[60,53]. While both of these molecules are potentially hazardous, they can be safely studied in the current laboratory setup if standard safety practices and those specific to the molecules are followed[62,63].

Dimethyl ether's rotational transitions have been observed between 38 GHz and 2100 GHz, making it an ideal molecule to study with the current signal generator[64]. Acetic acid also has a large range, which includes 8.531 GHz to 364.432 GHz, which is also within the current system's parameters[65]. A future project could keep the system as is and study dimethyl ether and acetic acid.

As the system is being optimized and rotational transitions of a molecule are being studied, the simulation code can also be advanced. Completing the simulation will allow the user to input any desired condition and to see how the data would look with those conditions.

References

[1] Di-Jia Liu, Wing-Cheung Ho, and Takeshi Oka. "Rotational Spectroscopy of Molecular Ions Using Diode Lasers". In: *The Journal of Chemical Physics* 87.5 (1987), pp. 2442–2446.

[2] Eric Herbst and Ewine F Van Dishoeck. "Complex Organic Interstellar Molecules". In: *Annual Review of Astronomy and Astrophysics* 47 (2009), pp. 427–480.

[3] Rennan Barkana and Abraham Loeb. "In the beginning: the first sources of light and the reionization of the universe". In: *Physics Reports* 349.2 (2001), pp. 125–238. ISSN: 0370-1573. DOI: `https://doi.org/10.1016/S0370-1573(01)00019-9`. URL: `https://www.sciencedirect.com/science/article/pii/S0370157301000199`.

[4] M De Simone et al. "Seeds of Life in Space (SOLIS)-X. Interstellar Complex Organic Molecules in the NGC 1333 IRAS 4A Outflows". In: *Astronomy & Astrophysics* 640 (2020), A75.

[5] Je Dyson and Da Williams. *Physics of the Interstellar Medium*. 1980.

[6] Andrew L Mattioda et al. "Formation of Complex Organic Molecules (COMs) from Polycyclic Aromatic Hydrocarbons (PAHs): Implications for ISM IR Emission Plateaus and Solar System Organics". In: *ACS Earth and Space Chemistry* 4.12 (2020), pp. 2227–2245.

[7] M.K. Sharma et al. "Anomalous absorption in glycolaldehyde in a cosmic object". In: *New Astronomy* 45 (2016), pp. 45–47. ISSN: 1384-1076. DOI: `https://doi.org/10.1016/j.newast.2015.10.005`. URL: `https://www.sciencedirect.com/science/article/pii/S1384107615001256`.

[8] Nicolle EB Zellner, Vanessa P McCaffrey, and Jayden HE Butler. "Cometary Glycolaldehyde as a Source of Pre-RNA Molecules". In: *Astrobiology* 20.11 (2020), pp. 1377–1388.

[9] M.K. Sharma et al. "Anomalous Absorption in Glycolaldehyde in a Cosmic Object". In: *New Astronomy* 45 (2016), pp. 45–47. ISSN: 1384-1076. DOI: `https://doi.org/10.1016/j.newast.2015.10.005`. URL: `https://www.sciencedirect.com/science/article/pii/S1384107615001256`.

[10] Susanna L Widicus Weaver et al. "Millimeter-Wave and Vibrational State Assignments for the Rotational Spectrum of Glycolaldehyde". In: *The Astrophysical Journal Supplement Series* 158.2 (2005), p. 188.

[11] Peter H Siegel. "THz Instruments for Space". In: *IEEE Transactions on Antennas and Propagation* (2007), pp. 2957–2965.

[12] D. Saeedkia. "1 - Optoelectronic Techniques for the Generation and Detection of Terahertz Waves". In: *Handbook of Terahertz Technology for Imaging, Sensing and Communications*. Ed. by Daryoosh Saeedkia. Woodhead Publishing Series in Electronic and Optical Materials. Woodhead Publishing, 2013, pp. 3–27. ISBN: 978-0-85709-235-9. DOI: `https://doi.org/10.1533/9780857096494.1.3`. URL: `https://www.sciencedirect.com/science/article/pii/B978085709235950001X`.

[13] Duncan V. Mifsud et al. "The Role of Terahertz and Far-IR Spectroscopy in Understanding the Formation and Evolution of Interstellar Prebiotic Molecules". In: *Frontiers in Astronomy and Space Sciences* 8 (2021). URL: `https://www.frontiersin.org/articles/10.3389/fspas.2021.757619`.

[14] "Spectroscopy 101 - How Absorption and Emission Spectra Work". In: (2021). URL: `https://webbtelescope.org/contents/articles/spectroscopy-101--how-absorption-and-emission-spectra-work`.

[15] Edinburgh Instruments. *Terahertz Molecular Lasers - Introduction Applications.* 2021. URL: `https://www.edinst.com/us/terahertz-molecular-lasers-introduction-applications/`.

[16] Rebecca Ljungren. "Higher Ground". In: (2018).

[17] I. Kleiner. “Asymmetric-Top Molecules Containing One Methyl-Like Internal Rotor: Methods and Codes for Fitting and Predicting Spectra”. In: *Journal of Molecular Spectroscopy* 260.1 (2010), pp. 1–18. ISSN: 0022-2852. DOI: `https://doi.org/10.1016/j.jms.2009.12.011`. URL: `https://www.sciencedirect.com/science/article/pii/S0022285209002884`.

[18] Peter H Siegel. “THz for Space: The Golden Age”. In: *2010 IEEE MTT-S International Microwave Symposium*. 2010, pp. 816–819.

[19] Chemistry Libre Texts. *1.9: Essential Elements for Life*. 2022.

[20] “Sugar is Sweet Essential to Life- and It’s Probably in Deep Space”. In: (2018). Ed. by Rick Chen.

[21] Molly Sargen. “Biological Roles of Water: Why is Water Necessary for Life”. In: *Retrieved from Science in the news: https://sitn. hms. harvard. edu/uncategorized/2019/biologicalroles-of-water-why-is-water-necessary-for-life* (2019).

[22] UK National History Museum. “Eight Ingredients for Life in Space”. In: (). URL: `https://www.nhm.ac.uk/discover/eight-ingredients-life-in-space.html`.

[23] Chemistry Libre Texts. *Rotational Spectroscopy of Diatomic Molecules*. 2023.

[24] *The Parts of the Periodic Table*. URL: `https://www.angelo.edu/faculty/kboudrea/periodic/structure_mass.htm`.

[25] M.A. Koshelev et al. “Water Vapor Line Profile at 183-GHz: Temperature Dependence of Broadening, Shifting, and Speed-Dependent Shape Parameters”. In: *Journal of Quantitative Spectroscopy and Radiative Transfer* 262 (2021), p. 107472. ISSN: 0022-4073. DOI: `https://doi.org/10.1016/j.jqsrt.2020.107472`. URL: `https://www.sciencedirect.com/science/article/pii/S0022407320310001`.

[26] X Xin et al. “Terahertz Absorption Spectrum of Para and Ortho Water Vapors at Different Humidities at Room Temperature”. In: *Journal of applied physics* 100.9 (2006), p. 094905.

[27] URL: `https://www.asiaa.sinica.edu.tw/research/_img/icsm_agb.jpg`.

[28] Wikipedia. *Glycolaldehyde*. 2023.

[29] Yuko Kawaguchi. "Panspermia Hypothesis: History of a Hypothesis and a Review of the Past, Present, and Future Planned Missions to Test This Hypothesis". In: *Astrobiology: From the Origins of Life to the Search for Extraterrestrial Intelligence*. Ed. by Akihiko Yamagishi, Takeshi Kakegawa, and Tomohiro Usui. Singapore: Springer Singapore, 2019, pp. 419–428. DOI: `10.1007/978-981-13-3639-3_27`. URL: `https://doi.org/10.1007/978-981-13-3639-3_27`.

[30] L. Reboussin et al. "Grain-Surface Reactions in Molecular Clouds: The Effect of Cosmic Rays and Quantum Tunnelling". In: *Monthly Notices of the Royal Astronomical Society* 440.4 (2014), pp. 3557–3567. ISSN: 0035-8711. DOI: `10.1093/mnras/stu462`. eprint: `https://academic.oup.com/mnras/article-pdf/440/4/3557/3858119/stu462.pdf`. URL: `https://doi.org/10.1093/mnras/stu462`.

[31] Jan M Hollis et al. "Green Bank Telescope Observations of Interstellar Glycolaldehyde: Low-Temperature Sugar". In: *The Astrophysical Journal* 613.1 (2004), p. L45.

[32] Cristina Puzzarini and Vincenzo Barone. "The Challenging Playground of Astrochemistry: An Integrated Rotational Spectroscopy – Quantum Chemistry Strategy". In: *Phys. Chem. Chem. Phys.* 22 (12 2020), pp. 6507–6523. DOI: `10.1039/D0CP00561D`. URL: `http://dx.doi.org/10.1039/D0CP00561D`.

[33] "Section 8d Cosmology: Doppler Red-Shift". In: ().

[34] dia Britannica Encyclopæ et al. *Spectroscopy*. 2015.

[35] Xiaojian Fu et al. "Applications of Terahertz Spectroscopy in the Detection and Recognition of Substances". In: *Frontiers in Physics* (2022), p. 427.

[36] Maureen Palmer et al. "ALMA Detection and Astrobiological Potential of Vinyl Cyanide on Titan". In: *Science Advances* 3 (July 2017), e1700022. DOI: `10.1126/sciadv.1700022`.

[37] George Gejo, Wilson Runcy, and Joy Jithin. “Chapter 3 - Ultraviolet Spectroscopy: A Facile Approach for the Characterization of Nanomaterials”. In: *Spectroscopic Methods for Nanomaterials Characterization*. Ed. by Sabu Thomas et al. Micro and Nano Technologies. Elsevier, 2017, pp. 55–72. ISBN: 978-0-323-46140-5. DOI: `https://doi.org/10.1016/B978-0-323-46140-5.00003-0`. URL: `https://www.sciencedirect.com/science/article/pii/B9780323461405000030`.

[38] Brian Drouin. “Molecular Spectroscopy”. In: ().

[39] Chemistry Libre Texts. *13.2 Rotational Transitions Accompany Vibrational Transitions*. 2023.

[40] R Nave. “Moment of Inertia”. In: ().

[41] Gejo George, Runcy Wilson, and Jithin Joy. “Chapter 3 - Ultraviolet Spectroscopy: A Facile Approach for the Characterization of Nanomaterials”. In: *Spectroscopic Methods for Nanomaterials Characterization*. Ed. by Sabu Thomas et al. Micro and Nano Technologies. Elsevier, 2017, pp. 55–72. ISBN: 978-0-323-46140-5. DOI: `https://doi.org/10.1016/B978-0-323-46140-5.00003-0`. URL: `https://www.sciencedirect.com/science/article/pii/B9780323461405000030`.

[42] R Nave. “The Interaction of Radiation with Matter”. In: ().

[43] I. Wilke. “Terahertz Spectroscopy Applications”. In: *Encyclopedia of Analytical Science (Third Edition)*. Ed. by Paul Worsfold et al. Third Edition. Oxford: Academic Press, 2017, pp. 1–5. ISBN: 978-0-08-101984-9. DOI: `https://doi.org/10.1016/B978-0-08-101983-2.12094-8`. URL: `https://www.sciencedirect.com/science/article/pii/B9780081019832120948`.

[44] Joel L. Bigman and Karen A. Reinhardt. “Chapter 11 - Monitoring of Chemicals and Water”. In: *Handbook of Silicon Wafer Cleaning Technology (Third Edition)*. Ed. by Karen A. Reinhardt and Werner Kern. Third Edition. William Andrew Publishing, 2018, pp. 619–657. ISBN: 978-0-323-51084-4. DOI: `https://doi.org/10.1016/B978-`

0-323-51084-4.00011-3. URL: `https://www.sciencedirect.com/science/article/pii/B9780323510844000113`.

[45] Sabu Thomas et al. *Spectroscopic Methods for Nanomaterials Characterization.* Vol. 2. Elsevier, 2017.

[46] Chemistry Libre Texts. *The Beer-Lambert Law.* 2023.

[47] R Nave. "Rotational Spectra". In: ().

[48] Sabrina Zinn et al. "High-Resolution Rotational Spectroscopy Study of the Smallest Sugar Dimer: Interplay of Hydrogen Bonds in the Glycolaldehyde Dimer". In: *Angewandte Chemie International Edition* 55.20 (2016), pp. 5975–5980.

[49] Edinburgh Instruments. *What is a Spectrometer.* 2023. URL: `https://www.edinst.com/blog/what-is-a-spectrometer/`.

[50] Laser Lab Source. "Spectrometer Basics". In: (2023). URL: `https://www.laserlabsource.com/Spectrometers/spectrometer-basics/`.

[51] *Types of Spectra: Continuous, Emission, and Absorption.* 2021. URL: `https://webbtelescope.org/contents/media/images/01F8GF8DK2PRY4FP9DA2XPQC8S`.

[52] Michel Gué lin and Jose Cernicharo. "Organic molecules in interstellar space: Latest advances". In: *Frontiers in Astronomy and Space Sciences* 9 (2022), p. 787567.

[53] National Center for Biotechnology Information. "PubChem Compound Summary for CID 178, Acetic Acid"". In: (2023).

[54] *CHEBI: 15368.* 2015. URL: `https://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:15368`.

[55] *Safty Data Sheet: Acrolein.* 2023.

[56] Kozo Inuzuka. "Electronic and Vibrational States of Acrolein". In: *Bulletin of the Chemical Society of Japan* 34.5 (1961), pp. 729–732.

[57] Karl-Heinz Dostert et al. “Adsorption of Acrolein, Propanal, and Allyl Alcohol on Pd (111): A Combined Infrared Reflection–Absorption Spectroscopy and Temperature Programmed Desorption Study”. In: *Physical Chemistry Chemical Physics* 18.20 (2016), pp. 13960–13973.

[58] Manfred Winnewisser et al. “Ground State Centrifugal Distortion Constants of Trans-Acrolein, CH2 = CH — CHO from the Microwave and Millimeter Wave Rotational Spectra 1,2”. In: *Zeitschrift für Naturforschung A* 30.8 (1975), pp. 1001–1014. DOI: `doi:10.1515/zna-1975-0814`. URL: `https://doi.org/10.1515/zna-1975-0814`.

[59] Rebecca Trager. “Dimethyl Ether Found in a Planet-Forming Disc for the First Time”. In: (2022).

[60] Manfred Mü ller and Ute Hü bsch. “Dimethyl ether”. In: *Ullmann’s encyclopedia of industrial chemistry* (2000).

[61] Fabrizio Puletti et al. “Large Prebiotic Molecules in Space: Photophysics of Acetic Acid and Its Isomers,” in: *Monthly Notices of the Royal Astronomical Society* 402.3 (2010), pp. 1667–1674. ISSN: 0035-8711. DOI: `10.1111/j.1365-2966.2009.16053.x`. eprint: `https://academic.oup.com/mnras/article-pdf/402/3/1667/3119924/mnras0402-1667.pdf`. URL: `https://doi.org/10.1111/j.1365-2966.2009.16053.x`.

[62] *Safety Data Sheet: Acetic Acid*. 2021.

[63] *Safty Data Sheet: Dimethyl Ether*. 2019.

[64] CP Endres et al. “Dimethyl Ether: Laboratory Spectra Up to 2.1 THz-Torsion-Rotational Spectra Within the Vibrational Ground State”. In: *Astronomy & Astrophysics* 504.2 (2009), pp. 635–640.

[65] V Ilyushin, I Kleiner, and Francis J Lovas. “Microwave Spectra of Molecules of Astrophysical Interest. XXVI. Acetic acid (CH 3 COOH)”. In: *Journal of Physical and Chemical Reference Data* 37.1 (2008), pp. 97–265.