Terahertz Gas-Phase Spectroscopy for Interstellar Applications

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In
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Abstract

Interstellar molecules are a significant resource that provide insight to characterize the interior of molecular clouds. Since these molecules are hundreds of lightyears away, samples cannot be taken to identify them. However, molecular spectroscopy can be performed to determine spectral lines of known molecules on Earth to compare with the emission lines captured through radio astronomy. This paper presents the design and construction of a gas-phase laboratory spectrometer utilizing terahertz radiation to measure the spectral lines of water and glycolaldehyde, a common complex organic molecule found in the interstellar medium.

Acknowledgements

I would like to acknowledge the following people for their contributions to this project:

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1. Introduction

The interstellar medium (ISM) provides insight into understanding the origin and evolution of life in the universe, particularly through complex organic molecules (COMs). One COM that is prominently studied in astrochemistry is glycolaldehyde (CH_2OHCHO) since it is the simplest monosaccharide sugar and reacts with propenal to form ribose, which is found in ribonucleic acid (RNA), a molecule fundamental to life [1]. Interstellar molecules are a significant resource that allows for the interior of molecular clouds to be investigated and characterized by its gaseous composition. Since these molecules are hundreds of lightyears away, scientists are unable to take samples of the ISM to determine its composition. However, spectral lines from these gases can be recorded using radio astronomy and compared with spectroscopic laboratory measurements of known molecules to identify these molecules through their respective spectral signatures. Over the last 80 years, the composition of the ISM has been explored through radio astronomy and rotational spectroscopy and over 200 molecules have been detected [2]. As more molecules are searched for in the cosmos, there are some complicated molecules that are more difficult to determine due to their weaker spectral signatures; therefore, precise spectroscopic laboratory measurements are essential for identifying molecules in the ISM. Future applications of these measurements could include the creation of a spectroscopic database that artificial intelligence could utilize to analyze large data sets from radio telescopes.

1.1 Goals of the Project

The goal of this project was to design and construct a gas-phase laboratory spectrometer utilizing terahertz radiation to measure the spectral lines of water and glycolaldehyde, a common complex organic molecule found in the interstellar medium. The following research objectives were set to achieve this goal:

1. Build a preliminary spectrometer to become familiar with equipment.

The key components for a direct absorption spectrometer were assembled using equipment at the Laboratory for Education and Application Prototypes (LEAP) facility. The optical components of the system were then aligned to collimate and focus the terahertz radiation.

2. Measure the spectral line of water to confirm the system works.

LABVIEW scripts were developed to automate the data collection process and spectral analysis was performed using IgorPRO. Frequency sweeps were taken at low pressure to observe the spectral line of water. After analyzing data taken with the preliminary spectrometer, its performance was evaluated to provide suggestions for designing a new spectrometer.

3. Design more comprehensive set-up and purchase new equipment.

Using the suggestions based on the preliminary spectrometer, the dimensions and material for a new absorption cell were determined to optimize interactions between terahertz radiation and gas-phase molecules. Calculations were also performed to minimize power loss through the cell.

4. Measure the spectral line of water and glycolaldehyde using the new spectrometer.

Once the new absorption cell was built, frequency sweeps were taken over the same frequency range to observe the spectral line of water. While glycolaldehyde was unable to be measured due to long lead times for equipment purchased, we were able to successfully measure the high-resolution spectra of water.

2. Background

In this section, the terahertz region of the electromagnetic spectrum and its role in molecular spectroscopy are explained. Applications of terahertz spectroscopy are also presented.

2.1 THz Regime of the Electromagnetic Spectrum

The terahertz (THz) region of the electromagnetic spectrum refers to high frequencies between 100 GHz and 10 THz or wavelengths between 3 mm and 30 μm [3]. This area of the electromagnetic spectrum overlaps with both the infrared and microwave regions and was not utilized until the 1990s due to the lack of sufficient THz sources and detectors; for this reason, the overlap between the infrared and microwave regions is known as the THz gap. As more research was conducted in this spectral range, advancements in THz generation and detection emerged, leading to improvements in THz technology and a wide variety of applications, including the study of rotational and vibrational molecular states through THz spectroscopy [4]. Since many molecules exhibit rotational and vibrational motion in the THz band, THz spectroscopy is a valuable tool to observe the interaction between radiation and molecules [5].

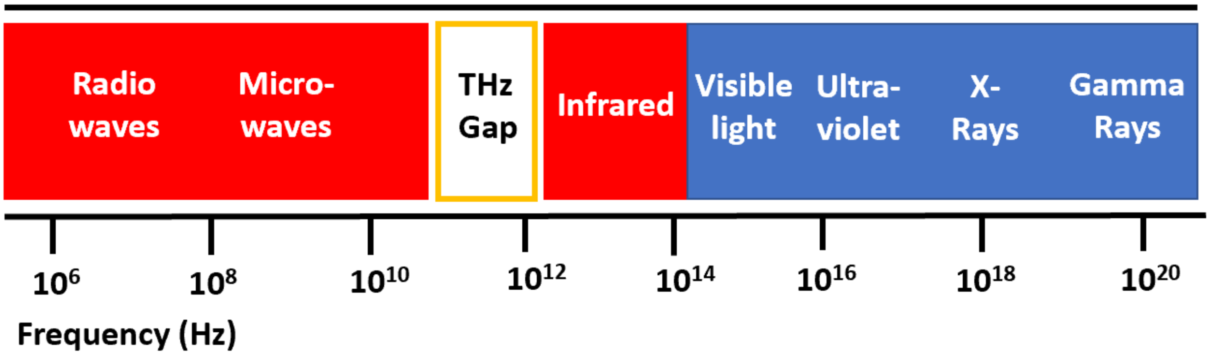

Figure 1: Regions of the electromagnetic spectrum by frequency. The THz gap is shown between the microwave and infrared regions and covers a frequency range of 100 GHz to 10 THz.

2.2 Interaction of Radiation and Matter

Radiation is the emission or transmission of energy in the form of electromagnetic waves or particles that travels through a medium. The interaction between radiation and matter can be explained through the semiclassical Schrödinger model [6]. In a two-level system with upper state wavefunction Ψ_1 and lower state wavefunction Ψ_0, the energy levels of molecules can be obtained through the solution of the time-independent Schrödinger equation shown below:

$$\hat{H}\Psi_1 = E\Psi_0 \tag{1}$$

where Ĥ is the Hamiltonian, E is energy, and radiation is treated classically [6]. Two processes can occur to cause an energy transition between the two energy levels: 1) stimulated emission or 2) absorption. Stimulated emission occurs when radiation of a specific frequency interacts with a molecule in an upper energy level. The energy of the radiation is equivalent to the energy of the band gap, which causes a transition to a lower energy level. In contrast to stimulated emission, absorption occurs when radiation interacts with a molecule at a lower energy level. The energy is absorbed by the radiation, causing a transition to a higher energy level [6].

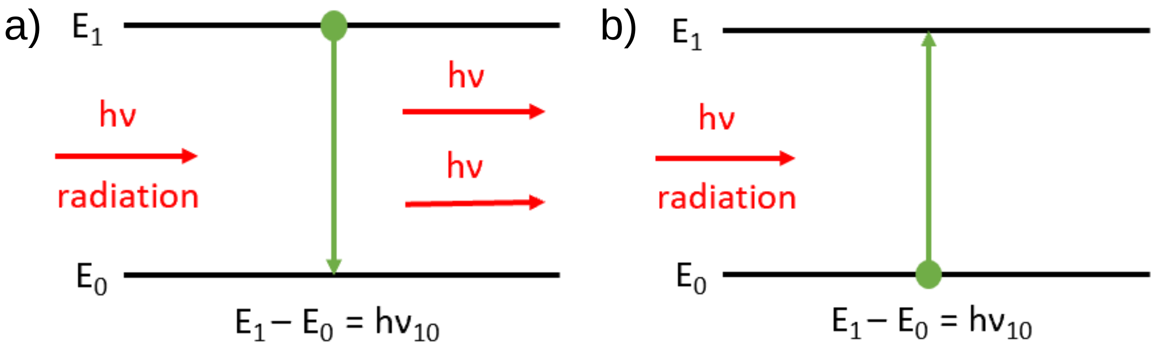

Figure 2: Stimulated emission (a) and absorption (b) in a two-level system.

2.3 Molecular Spectroscopy

Molecular spectroscopy refers to the absorption and emission of electromagnetic radiation by solid, liquid, or gas molecules. When these molecules undergo absorption or emission in the gas phase, molecular spectra can be observed in the rotational, vibrational, or electronic energy states [7]. In classical mechanics, rotational energy refers to the kinetic energy of a rotating body;

this concept remains relevant on the molecular level. To study the rotational states of a molecule, the rigid-rotor model is used, which assumes that the molecule is a rigid object with fixed bond lengths and no vibrations [8]. For simplicity, consider a rigid diatomic molecule with masses m_1 and m_2 separated by a distance r and rotating in the XYZ coordinate system. The model can be simplified by determining the reduced mass of the system, μ, to solve for its moment of inertia.

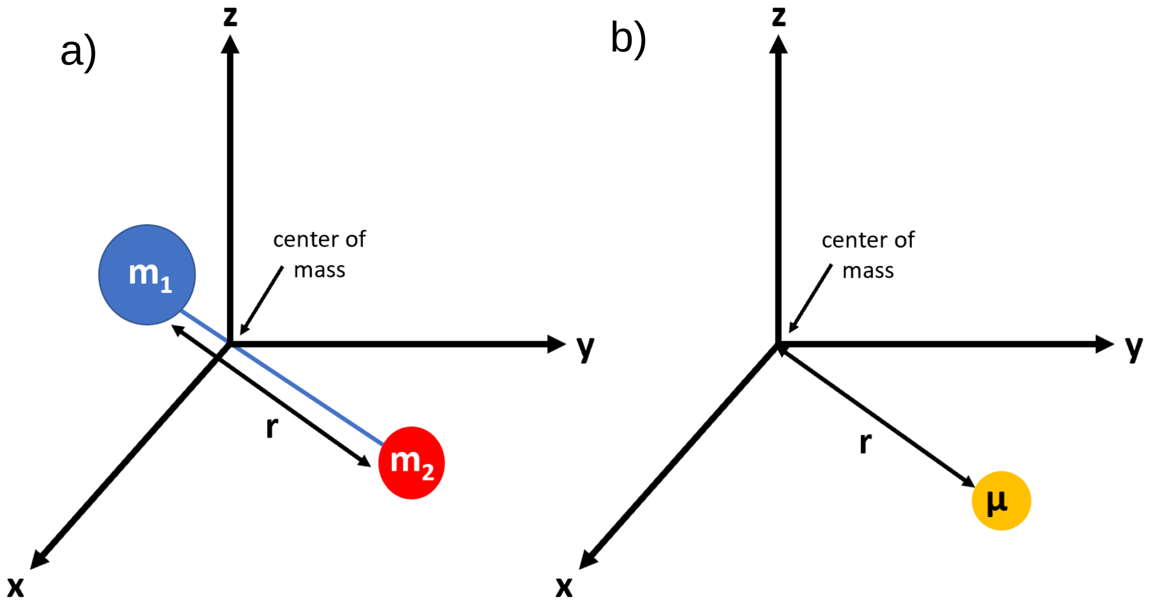

Figure 3: Diagrams of XYZ coordinate system for a) a diatomic molecule with masses m_1 and m_2 separated by distance r and b) the reduced mass model of the molecule simplified to one particle.

The moment of inertia of this molecule is shown below:

$$I = \mu r^2 = \frac{m_1 m_2}{m_1+m_2} r^2 \tag{2}$$

Angular momentum of the molecule can be represented by:

$$L = I\omega \tag{3}$$

where L is angular momentum and ω is angular velocity. By taking the summation of all components in the x, y, and z directions, angular momentum can be written as a matrix equation:

$$\begin{bmatrix} L_1 \\ L_2 \\ L_3 \end{bmatrix} = \begin{bmatrix} I_{xx} & I_{xy} & I_{xz} \\ I_{yx} & I_{yy} & I_{yz} \\ I_{zx} & I_{zy} & I_{zz} \end{bmatrix} \begin{bmatrix} \omega_x \\ \omega_y \\ \omega_z \end{bmatrix} \tag{4}$$

Principal axes of inertia are defined based on the symmetry of the molecule and are used to determine the principal moments of inertia, I_{xx}, I_{yy}, and I_{zz}, which show moment of inertia contributions in the x, y, and z directions. By analyzing the principal moments of inertia, the structure of the molecule can be obtained. If the principal moments are all unique, the molecule is an asymmetric top; if two principal moments are identical, the molecule is a symmetric top; and if all three moments are identical, the molecule is a spherical top [9].

2.4 Direct Absorption Spectroscopy

Absorption spectroscopy involves measuring how much radiation is absorbed over a specific frequency range. Radiation from a source is sent through a cell filled with a gas sample at a known pressure and the intensity of this radiation is measured by a detector. To measure the absorption, the transmitted intensity measured by the detector is compared to the incident intensity by Beer's Law:

$$I(\nu) = I_0 e^{-\alpha(\nu)L} \tag{5}$$

where $I(\nu)$ is the transmitted intensity, I_0 is the incident intensity, α is the absorption coefficient, and L is the length of the cell [10]. By analyzing the transmitted intensity as a function of frequency, a sharp dip in the spectrum called a spectral line or absorption line can be observed.

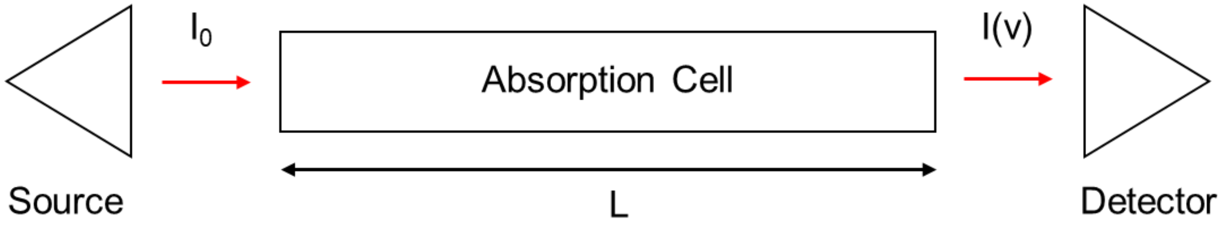

Figure 4: Diagram of direct absorption spectroscopy. A source emits radiation through an absorption cell of length L which is then received by a detector.

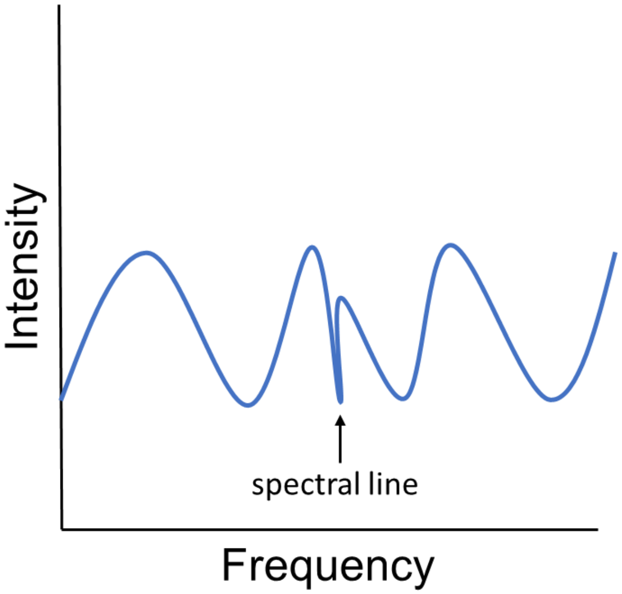

Figure 5: Intensity as a function of frequency. The sudden dip in the spectrum is a spectral line associated with a specific molecule and occurs due to absorption.

This feature is very narrow compared to the rest of the received signal, but when the scale is expanded, the spectral line can be defined by its width ($\nu_{1/2}$) and line-shape.

2.4.1 Line-Shape Functions

Line-shape functions describe the transition between energy states of a molecule. There are two categories of lines-shape functions: 1) homogeneous, where all molecules exhibit the same absorption spectra and 2) inhomogeneous, where molecules exhibit different spectra [6]. For gas-phase molecules, line-shapes are determined by Doppler broadening and pressure broadening. Doppler broadening is the widening of spectral lines due to the Doppler Effect and is categorized as inhomogeneous broadening. As absorption or emission occur, molecules have different velocities that shift the frequency of the incident radiation. In contrast, pressure broadening is a type of homogeneous broadening that occurs due to collisions between molecules. These collisions transfer energy between molecules which allows for transitions to occur within a wider frequency range [11].

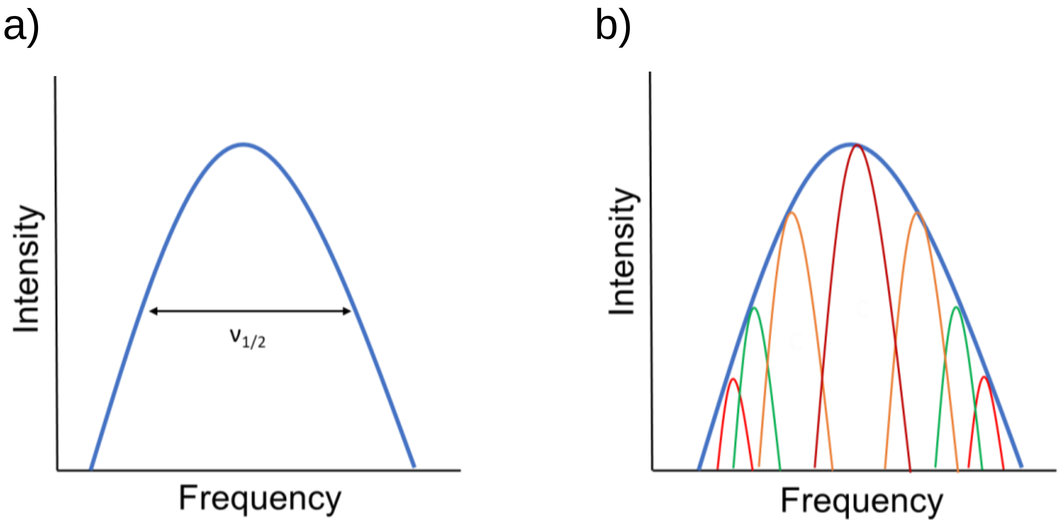

Figure 6: a) Homogeneous line-shape broadening and b) Inhomogeneous line-shape broadening. Inhomogeneous broadening has several lines overlapping due to molecules experiencing absorption at different frequencies.

The shape of homogeneous and inhomogeneous line-shapes can be one of three spectral line profiles: 1) Gaussian, 2) Lorentzian, or 3) Voigt. Inhomogeneous line-shapes commonly follow a Gaussian profile since the different molecular velocities follow a normal distribution. Homogeneous line-shapes follow a Lorentzian profile, typically with a narrower linewidth than a Gaussian profile [6]. A Voigt profile is a convolution of both Gaussian and Lorentzian profiles and is used when both homogeneous and inhomogeneous broadening occurs.

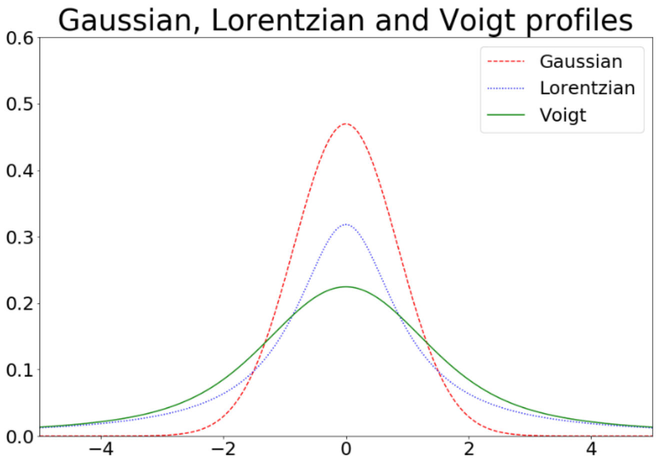

Figure 7: Spectral line profiles for homogeneous and inhomogeneous line-shapes. The dashed red curve is a Gaussian profile; the dashed blue line is a Lorentzian profile, and the green line is a Voigt profile [Wikimedia].

2.5 Applications of Terahertz Spectroscopy

THz technology has experienced rapid growth over the last few decades, particularly in the fields of astrochemistry and analytical chemistry. THz spectroscopy provides identifying information to characterize the chemical composition of gases detected on Earth and in space by analyzing absorption and emission lines of molecules. As a result, THz telescopes investigating the molecular composition of clouds in the interstellar medium and chemical sensing methods using THz radiation have emerged.

2.5.1 Radio Astronomy

Radio astronomy is a branch of astronomy that studies objects in space using radio frequencies. Celestial objects such as stars are comprised of several molecules that emit radiation at specific frequencies that can be detected from Earth and provide information regarding the composition of the star [12]. Looking into their composition gives insight into the formation of stars which involves the collapse of molecular gas clouds. The gases present in molecular clouds and other astronomical objects deep in space have spectral lines in the THz band that can be detected using THz telescopes [13]. Ground-based and space-based THz telescopes have been established to detect THz radiation from celestial objects to characterize their composition based on spectral analysis. Ground-based telescopes such as the High Elevation Antarctic Terahertz (HEAT) telescope in Antarctica and the Atacama Large Millimeter/sub-millimeter Array (ALMA) in Chile have been used to map the composition of molecular clouds in the nearby universe to gain a deeper understanding of star formation [13]. HEAT and ALMA are located in very dry climates

Figure 8: Antennas in the Atacama Large Millimeter/sub-millimeter Array in Chile [ALMA].

at high altitude, which prevents water vapor in the atmosphere from absorbing the radiation. These telescopes have one or more antennas to collect the radiation emitted by celestial objects and a receiver and amplifier to amplify the signal. Once the signal has been processed, the amplitude as a function of frequency indicates the spectral lines, which can be traced back to laboratory measurements of molecules to identify which molecules were detected.

2.5.2 Chemical Sensing

THz spectroscopy is also used to detect dangerous gases. Since there are numerous molecules that experience rotational and vibrational transitions in the THz range due to absorption or emission, the spectral lines produced by these interactions function as fingerprint information that can be used to identify which molecules are present. Dangerous gases can be detected remotely with a spectrometer using direct absorption spectroscopy. THz radiation is emitted between frequencies f_1 and f_3 to determine if a harmful gas with frequency f_2 is present as shown below [14]. If the gas is present, there will be a dip in the intensity of the radiation detected by the receiver at f_2.

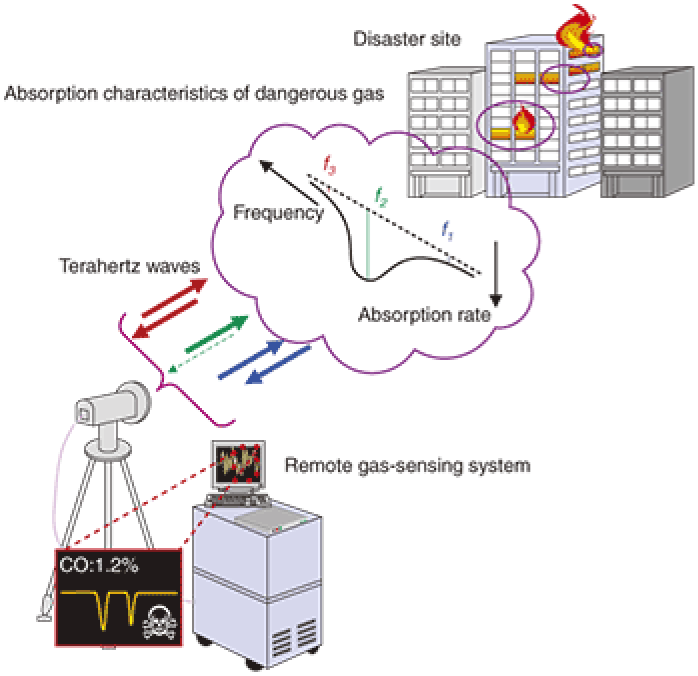

Figure 9: Remote sensing of dangerous gases through THz spectroscopy [14].

3. Methodology

The goal of this project was to design and construct a gas-phase laboratory spectrometer utilizing terahertz radiation to measure the spectral lines of water and glycolaldehyde. The following research objectives were set to achieve this goal:

1. Build a preliminary spectrometer to become familiar with equipment.
    a. Assemble key components for a direct absorption spectrometer using equipment at the LEAP facility.
    b. Align and optimize the optical components of the system.
2. Measure the spectral line of water to confirm the system works.
    a. Develop LABVIEW scripts to automate data collection process and spectral analysis.
    b. Perform frequency sweeps at low pressure to observe the spectral line.
3. Design more comprehensive set-up and purchase new equipment.
    a. Determine the dimensions and material used for a new absorption cell to optimize interactions between THz radiation and gas-phase molecules.
    b. Perform calculations to minimize power loss through the cell.
4. Measure the spectral line of water and glycolaldehyde using the new spectrometer.
    a. Perform frequency sweeps at low pressure to observe the spectral line of water.

3.1 Build Preliminary Spectrometer

The preliminary spectrometer system shown in Figure 10 was constructed with a 4.5-foot-long copper absorption cell, 1-inch in diameter. A gas handling cell was attached to the far left of the cell and a rotary vane vacuum pump was attached to the far right to create a near-vacuum pressure environment and draw the sample into the absorption cell. The pressure gauge on the vacuum pump was used to monitor the pressure inside the system. An RF signal generator was used in conjunction with a 6x frequency multiplier and emitter to generate the incoming THz signal near a frequency of 183 GHz corresponding to a water transition. Plano-convex lenses were used to collimate the incident signal through the cell and then focus the transmitted signal to the detector. The signal was then conditioned using a low noise preamplifier to eliminate high frequency noise and amplify the signal. The THz signal was amplitude modulated and a lock-in amplifier was then used to further eliminate noise. The signal was then recorded using a data acquisition card and processed using LABVIEW.

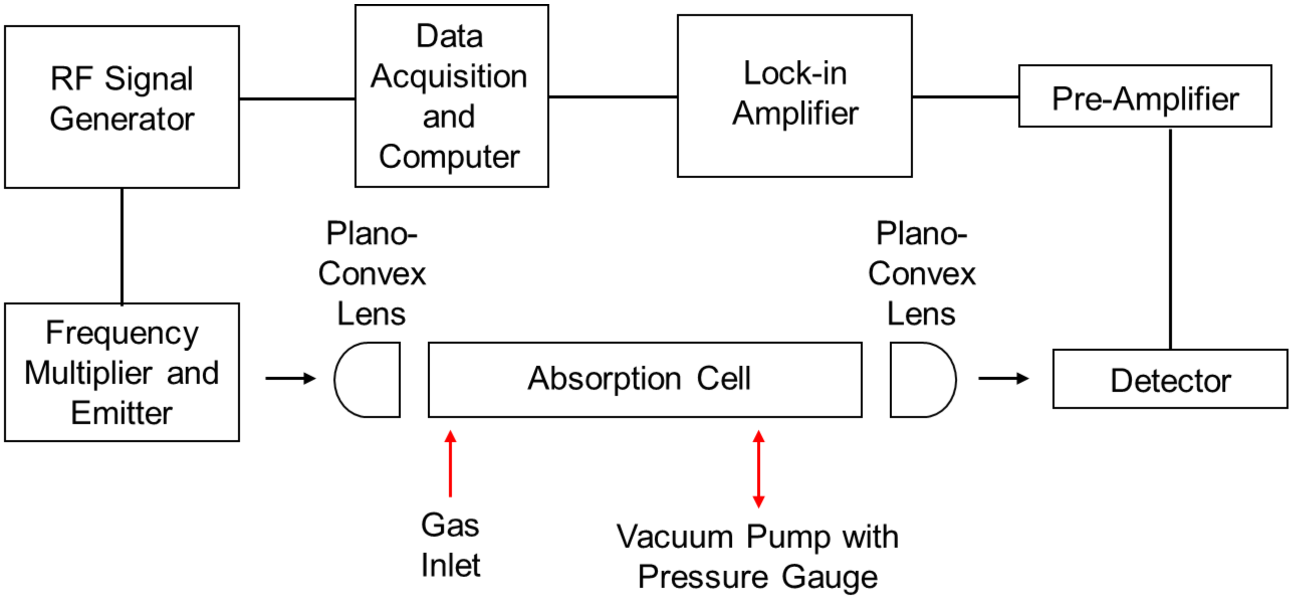

Figure 10: Preliminary spectrometer schematic using equipment from the LEAP facility.

3.1.1 Assemble Key Components for a Direct Absorption Spectrometer

When assembling a spectrometer, there are four main components, other than optics, to consider including an absorption cell, gas handling cell, pressure gauge, and a vacuum pump. Components from previous vacuum systems were available in the LEAP facility and were used to construct the absorption cell and add components onto the vacuum pump. Two copper pipes with Teflon endcaps and two gas inlets were connected to form the absorption cell for the system. A small vacuum chamber was used as a gas handling cell and was connected to the absorption cell with a rubber vacuum hose. The vacuum pump was then connected to the other side of the absorption cell using standard vacuum tubing.

3.1.2 Align and Optimize the Optical Components of the System

Once the spectrometer was constructed, the optical components of the system were laid out on the table and aligned by sight. Since the frequency multiplier chain and detector are both sensitive to electro-static discharge (ESD), ESD wrist straps were used to carefully position them. Two 2-inch plano-convex Teflon lenses with 75 mm focal lengths were placed on opposite sides of the absorption cell to allow radiation from the emitter, with a 13-degree horn angle (WR-5.1), to collimate through the cell and then focus down to the detector. The lenses were each placed approximately 3.46 cm from the source or detector respectively to allow the radiation to expand to the lens. Once all components were aligned by sight, each component was moved in the x, y, and z directions to optimize the transmitted intensity signal received by the detector.

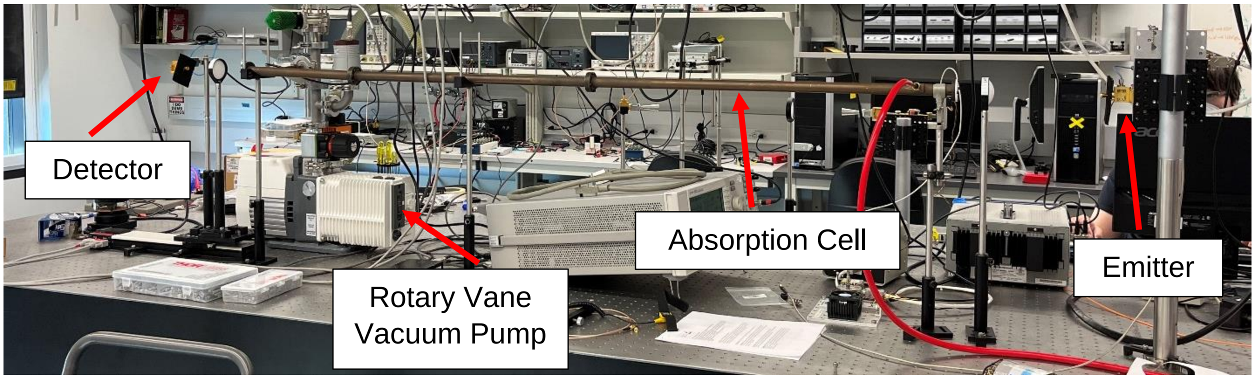

Figure 11: Preliminary spectrometer set-up.

3.2 Measure the Spectral Line of Water to Confirm System Works

To assess the effectiveness of the spectrometer, the spectral line of water was measured and compared to previously measured results found in literature. LABVIEW scripts were developed to perform frequency sweeps over a designated frequency range, including the frequency of the pure rotational transition of water (183.310 GHz) [15].

3.2.1 Develop Data Collection and Analysis Process

To facilitate the data collection process, a LABVIEW virtual instrument (VI) was developed to sweep through a specified frequency range and collect voltage response from the detector. The VI prompts the user for the start frequency, end frequency, and step size in GHz as well as the number of sweeps to perform; it then samples the intensity at the detector at a rate determined by the user and digitizes the data. Data was exported to IgorPRO for further analysis.

3.2.2 Perform Frequency Sweeps to Observe the Spectral Line

The system was pumped down to a few millitorr with the vacuum pump and then sealed off to determine if there were any leaks present in the system before introducing water. Using the LABVIEW script, frequency sweeps were taken between 183 GHz and 184 GHz with a step size of 0.001 GHz. A reference sweep was taken over this interval with no water present in the system to later be compared to the sweep taken with water. By taking these two frequency sweeps, the spectral line of water should be easily identifiable. Another set of frequency sweeps were taken on a smaller interval between 183.25 GHz and 183.40 GHz with a step size of 0.001 GHz.

3.3 Design More Comprehensive Set-up and Purchase New Equipment

After taking measurements with the initial spectrometer system, it became evident that the system was not optimized to take measurements of all gases at low pressure. The connections between the cell, pressure gauge, and holding cell were not properly sealed to prevent leaks in the system, which led to measurements becoming significantly pressure broadened to the point where the spectral line was indistinguishable. Additionally, the absorption cell was not ideal to take spectra of corrosive gases since there could be chemical interactions that could deteriorate the cell or pose safety hazards. The diameter and length of the cell could also be optimized to increase the number of interactions between the incident radiation and the molecules. These factors were all taken into consideration while designing a new spectrometer.

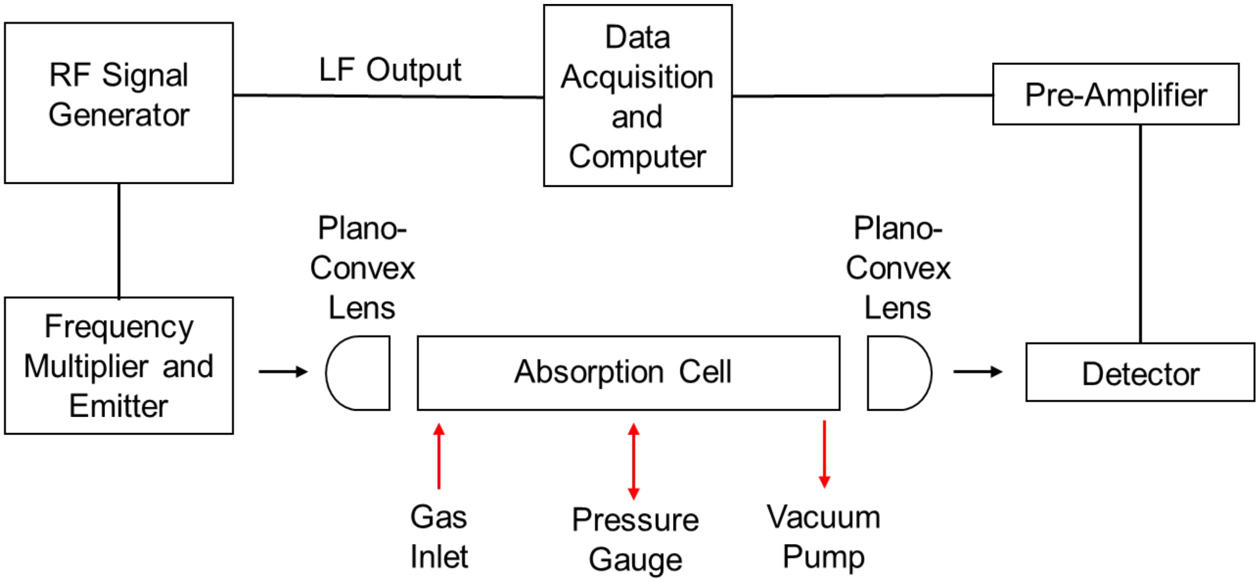

Figure 12: Final spectrometer schematic with absorption cell components purchased from ACE Glass.

3.3.1 Determine Dimensions and Material Used for a New Absorption Cell

To increase the number of interactions in the cell, the length of the cell was extended to 5.5 feet. According to Beer's Law, longer path length corresponds to more molecules in the path of radiation, which leads to more interactions and thus, higher levels of absorption. Other optical elements such as rooftop reflectors were considered to create a double pass absorption cell, which would have extended the optical path length to 11 feet but were not implemented due to time restraints. The diameter of the cell was also extended to 4 inches to increase the area of radiation that collimates through the cell to increase the number of interactions and reduce losses due to diffraction. To eliminate the risk of corrosion and safety hazards associated with using a copper absorption cell, the new absorption cell was designed to be made of glass with Teflon end caps.

As for the layout of the absorption cell, three 6-inch reducing tees and two 2-foot straight process pipes were chosen to construct the cell. The design consisted of two reducing tees on the end of the cell, each clamped to a straight process pipe, and the two process pipes were connected to a reducing tee in the center. The reason behind this design was to connect the pressure gauge to the reducing tee in the center of the cell to ensure that it was reading the pressure inside the cell. The other two reducing tees were used to connect the vacuum pump and the gas holding cell.

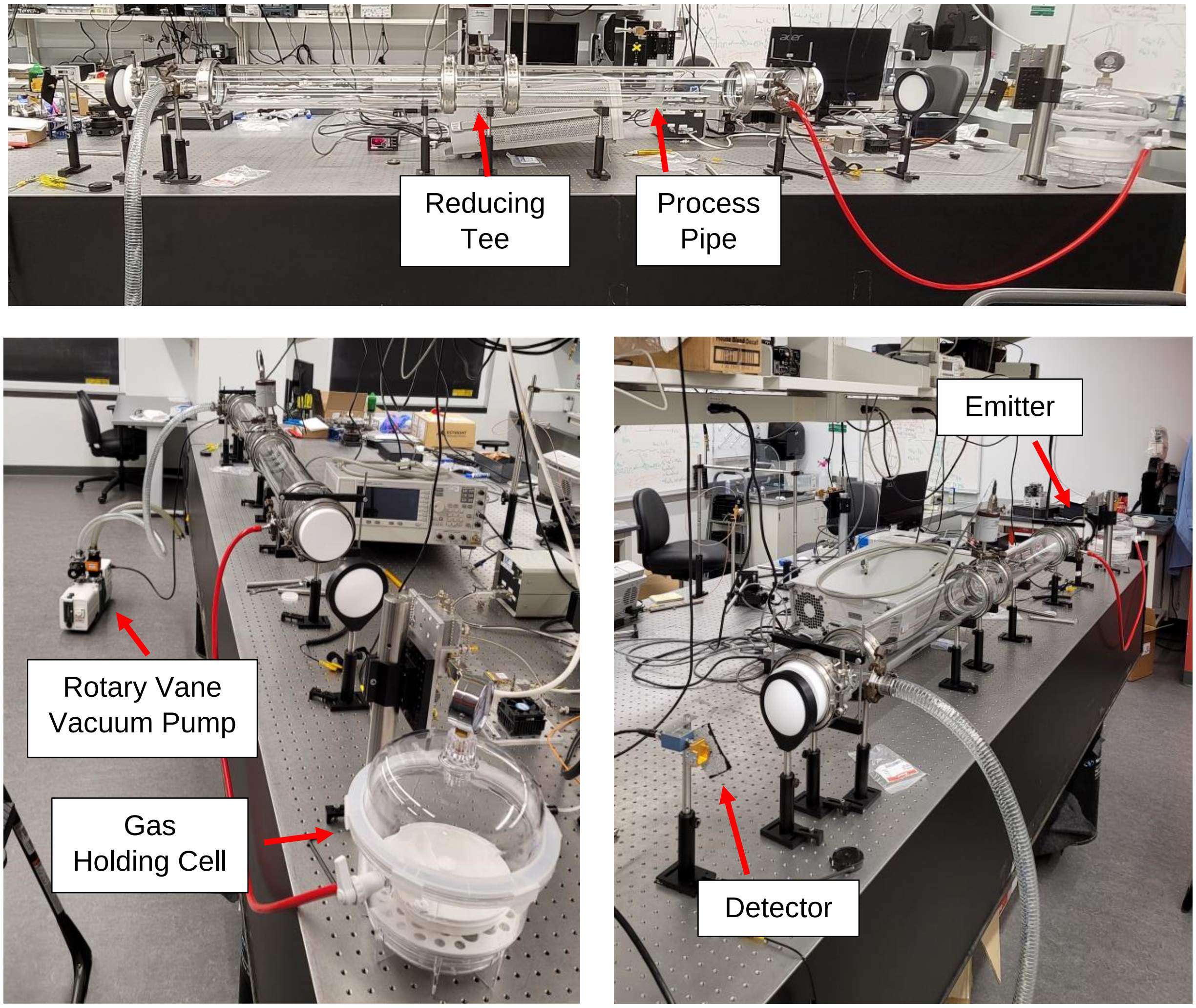

Figure 13: Final spectrometer set-up from a) the front, b) emitter side, and c) detector side.

3.3.2 Perform Calculations to Minimize Power Loss through the Cell

To ensure the integrity of the signal, little to no radiation can expand beyond the diameter of the cell to guarantee that the detector measures the full transmitted intensity of the radiation. The spread of the beam from the emitter to the lens was determined to be 26 mm given the geometry of the horn. As the beam collimates through the cell, it diverges at an angle determined by the wavelength of the beam over the diameter of the beam at the lens shown below:

$$\theta \sim \frac{\lambda}{D} \tag{6}$$

For measurements taken at 183 GHz (1.635 mm), the beam expands at an angle of 0.0628 degrees. The expansion of the beam is shown in Figure 14. Using trigonometry, the length that the beam expands to in millimeters can be calculated as shown below:

$$L = 2\left(1676\, tan\, \left(\frac{\theta}{2}\right) + 13\right) = 27.84\, mm \tag{7}$$

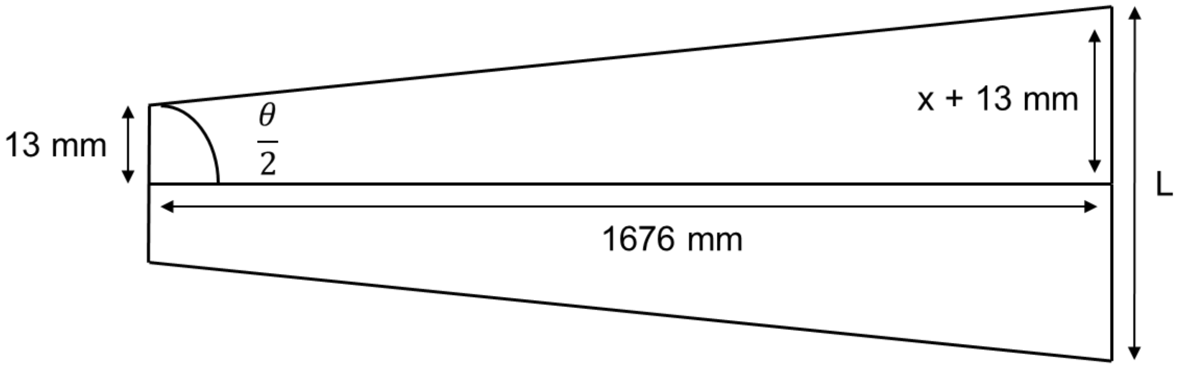

Figure 14: Expansion of a collimated beam through the absorption cell. The beam has a diameter of 26 mm at the first lens on the left and expands at a 0.0628-degree angle to 27.84 mm at the second lens on the right.

Since the diameter of the beam at the end of the absorption cell is less than the diameter of the cell, we expect there to be no power loss through the cell caused by beam expansion.

3.4 Measure the Spectral Line of Water with the New Spectrometer

To test the newly constructed spectrometer, the spectral line of water was re-measured. The same data collection process was used to perform frequency sweeps over a specified frequency range and step size.

3.4.1 Perform Frequency Sweeps to Re-measure the Spectral Line of Water

The new spectrometer was pumped down to a few millitorr with the vacuum pump and then sealed off to determine if there were any leaks present in the system before introducing water. Clamps were tightened and vacuum grease was used with the gaskets to create a tighter seal between sections of the absorption cell. Once it was confirmed that there were no leaks in the system, frequency sweeps were taken between 183 GHz and 184 GHz with a step size of 0.001

GHz. Once the spectral line was identified, the data was exported to IgorPRO to characterize the linewidth and broadening factors.

4. Results

This section explains and analyzes the results from the two spectrometer systems. The first subsection delves into the results from the preliminary spectrometer system and the second subsection displays the results from the final spectrometer system and compares them to the preliminary system.

4.1 Preliminary Spectrometer Results

Frequency sweeps between 183 GHz and 184 GHz were taken to locate the absorption line of water which was expected to be at 183.310 GHz. Two sets of data were acquired using the LABVIEW script, one with water in the system and one without water in the system. These results are shown in Figure 15. A sharp dip in the signal with water was expected at 183.310 GHz but was not apparent. The signal with water (sample signal) and the signal without water (reference signal)

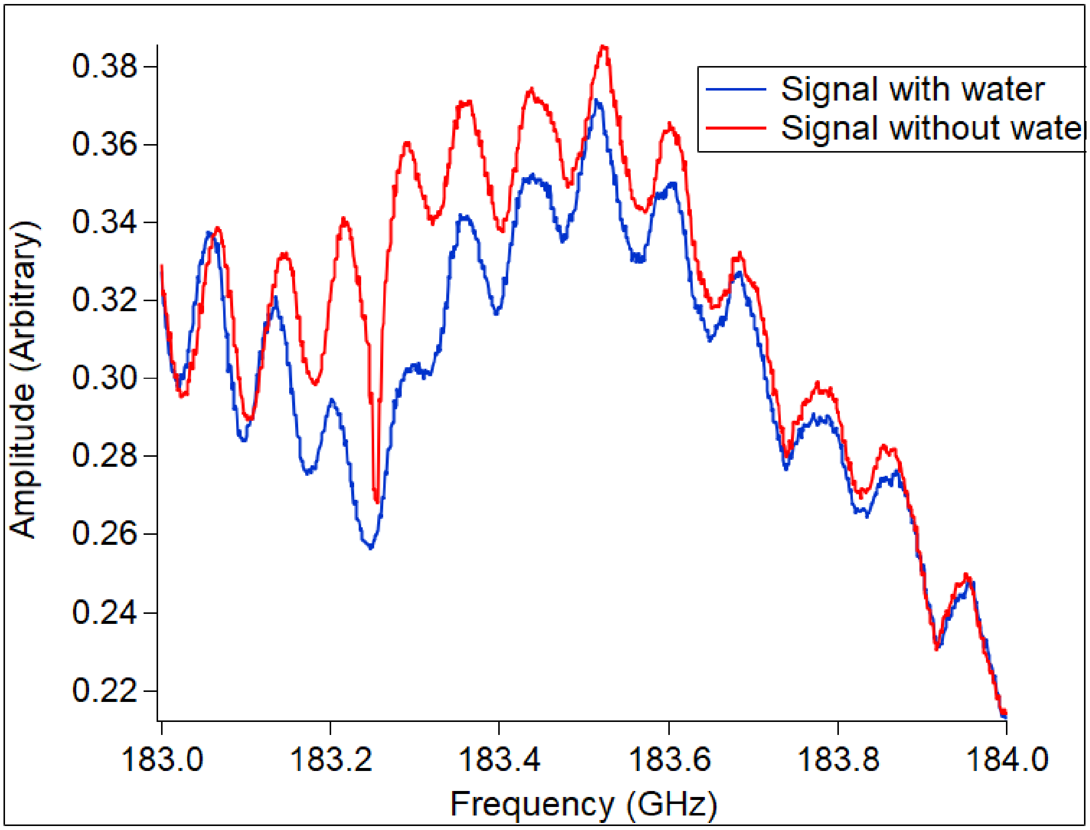

Figure 15: Spectra taken from 183 GHz to 184 GHz with a step size of 0.001 GHz. The general patterns of both signals resemble each other closely and do not clearly indicate the spectral line of water.

resembled each other closely until 183.10 GHz where the amplitude of the sample signal was consistently less than the amplitude of the reference signal. The curvature of the two signals remained consistent throughout the rest of the data. Since it was not clear if the spectral line of water was captured over this frequency range, a second set of data was taken between 183.25 GHz and 183.40 GHz to zoom in on the area that the spectral line is expected to be observed at. These results are shown in Figure 16. The curvature of the two signals remained consistent throughout the data and the frequency at which the spectral line of water was expected at was still indistinguishable. The pressure at which the results were acquired at with water in the system were a few millitorr as shown on the pressure gauge, which theoretically is a low enough pressure to produce a sharp spectral line on the order of 1 MHz wide. Additionally, once measurements were taken and the vacuum was powered off, the pressure inside the absorption cell increased rather quickly, indicating that there were leaks in the system. For these reasons, the results indicate that the spectral line was pressure broadened.

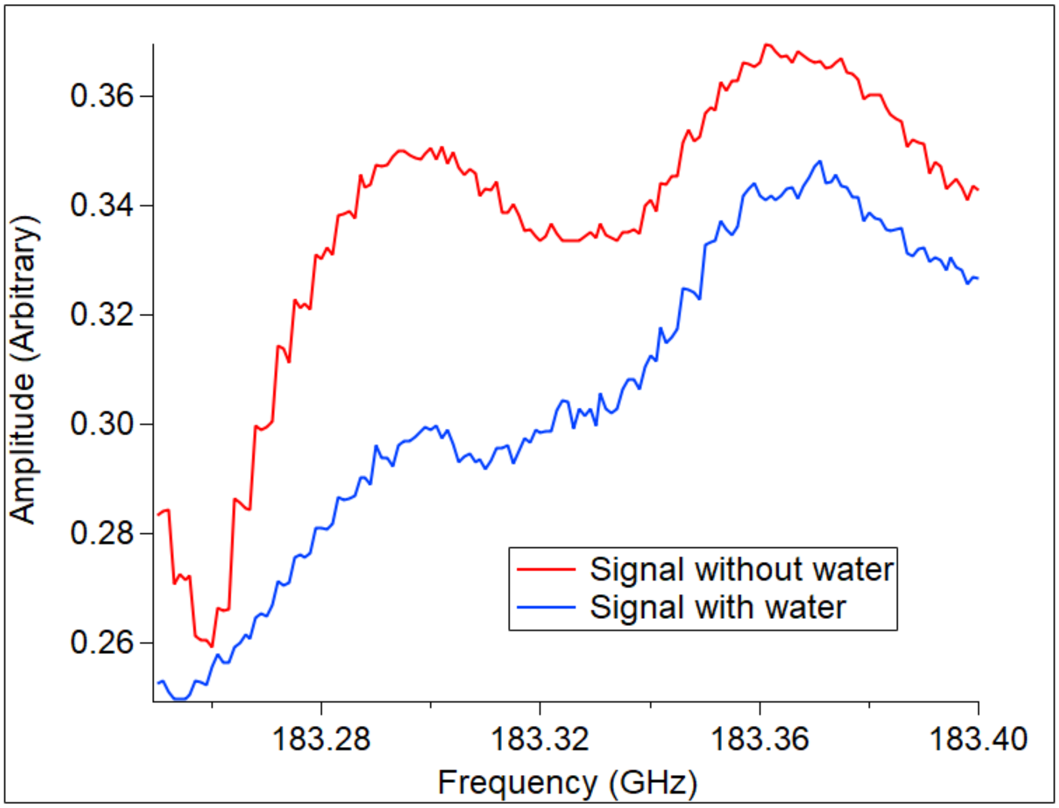

Figure 16: Spectra taken from 183.25 GHz to 183.40 GHz with a step size of 0.001 GHz. The general patterns of both signals resemble each other closely and do not clearly indicate the spectral line of water.

4.2 Final Spectrometer Results

Frequency sweeps between 183.20 GHz and 183.40 GHz were taken to look for the spectral line of water with the newly built spectrometer. These results are shown in Figure 17. A sharp dip in the signal was observed at 183.316 GHz at a pressure of 0.7 mTorr, confirming that the spectral line of water was captured.

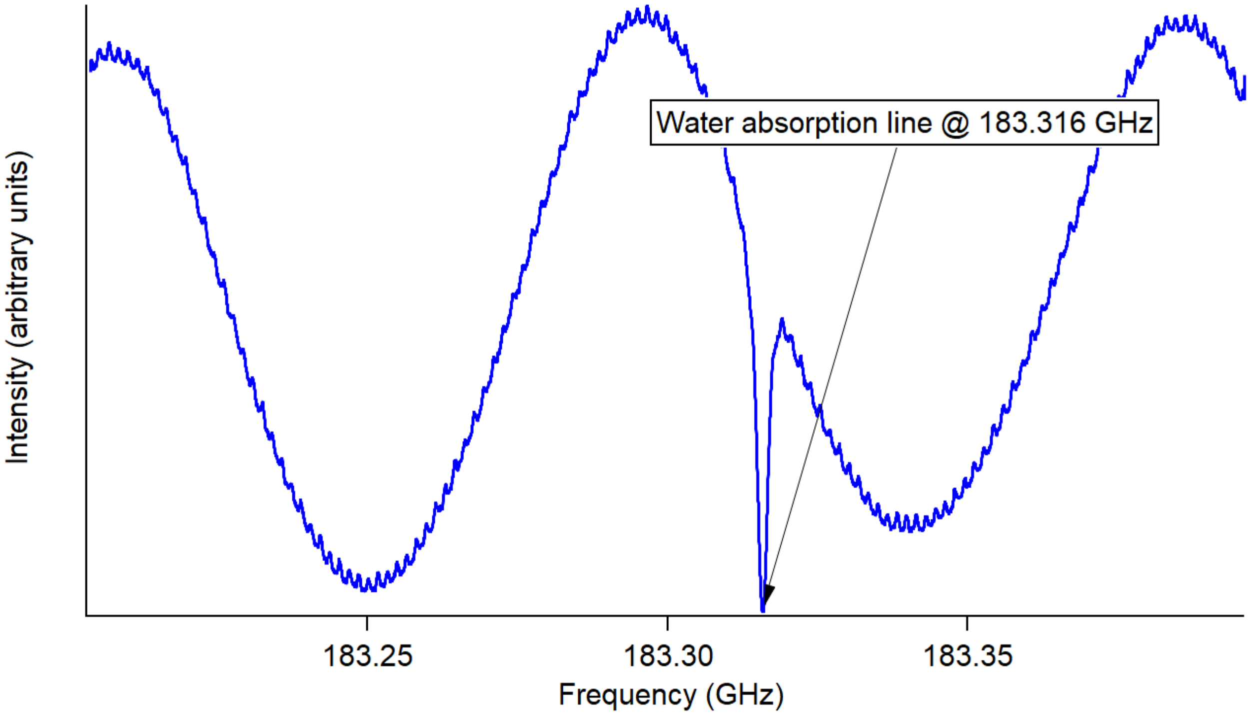

Figure 17: Spectra taken from 183.20 GHz to 183.40 GHz with a step size of 0.001 GHz. The spectral line of water was obtained at 183.316 GHz.

While the spectral line acquired with the final spectrometer was much more defined than the preliminary spectrometer, there were concerns that the pressure gauge was not displaying the correct pressure for two reasons: 1) the vapor pressure of water at 296 Kelvin is 20 torr, therefore the pressure of the system should not be lower than that if the cell is completely open to the water sample; and 2) the lowest pressure that the vacuum pump can achieve is 1.5 mTorr, which was lower than expected since only a mechanical roughing pump was used to create the vacuum. To investigate the accuracy of the pressure gauge, the spectral line was analyzed by applying line fits to characterize the contributions of both Doppler and pressure broadening.

The spectral line was isolated from the rest of the signal and was fit to a Voigt line profile to account for contributions from both Doppler and pressure broadening as shown in Figure 18.

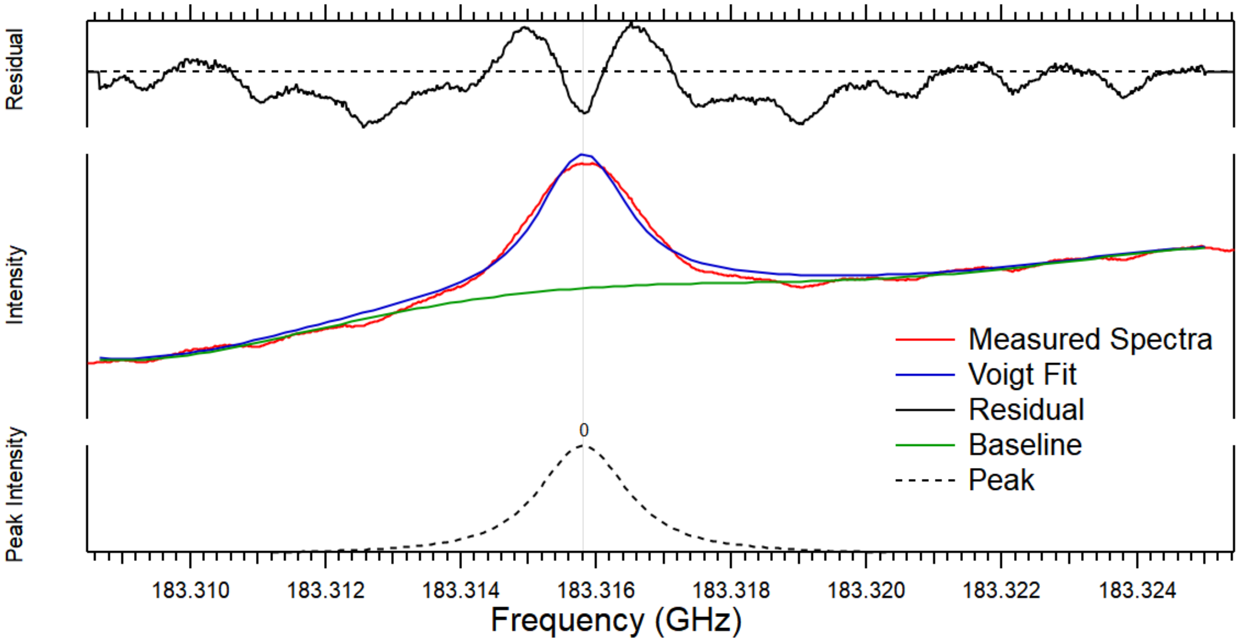

Figure 18: The spectral line of water fit to a Voigt profile over a frequency range of 183.308 GHz to 183.326 GHz.

The Doppler linewidth was calculated using

$$\Delta\nu_D = \frac{\nu}{c}\sqrt{\frac{2kTN_0 ln(2)}{M}} \tag{8}$$

where ν is the pure rotational transition frequency of water, c is the speed of light, k is the Boltzmann constant, N_0 is Avogadro's number, and M is the molecular weight of water. The linewidth due to Doppler broadening was determined to be 0.531 MHz and was inserted as a parameter for the Voigt fit to obtain the linewidth due to pressure broadening, which was found to be 1.385 ± 0.017 MHz. For water vapor molecules at a temperature of 296 Kelvin, the pressure broadening linewidth parameter is 20.55 ± 0.17 MHz/Torr. Using the pressure broadening linewidth from the Voigt profile $\Delta\nu_{Voigt}$ and this linewidth parameter, the pressure inside the absorption cell was able to be calculated as shown below:

$$p = \frac{\Delta\nu_{Voigt}}{20.55\ MHz/Torr} = 67.4\ mTorr \tag{9}$$

This value is almost two orders of magnitude greater than the value the pressure gauge was displaying, which confirms that the pressure gauge was not providing accurate readings.

5. Conclusions and Recommendations for Future Work

The goal of this project was to design and build a gas-phase laboratory spectrometer utilizing terahertz radiation to measure the spectral line of water and glycolaldehyde. Due to long lead times for equipment purchased for the final spectrometer, only the spectral line of water was successfully measured.

5.1 Conclusions

Both a preliminary and final spectrometer were designed and built to measure spectra of gas-phase molecules in the terahertz band. While the preliminary spectrometer was unable to successfully measure the pure rotational transition of water, the final spectrometer successfully captured the spectral line at 183.316 GHz. It was determined that the measurements made with both the preliminary and final spectrometer were pressure broadened. Pressure broadening was more prevalent in the preliminary spectrometer due to unsecure connections between components of the absorption cell in addition to inaccurate pressure gauge readings. The final spectrometer had more secure connections which reduced the rate at which pressure increased in the cell as well as narrowed the spectral line, making it easier to distinguish from the rest of the data. This indicates that the pressure gauge is in need of calibration.

5.2 Recommendations for Future Work

In the future, other interstellar molecules such as glycolaldehyde can be measured using the final spectrometer to provide laboratory measurements that can be referred to when analyzing spectral data from molecular clouds. These measurements can be stored in a database for artificial intelligence to utilize when analyzing large data sets from radio telescopes.

One problem with the final spectrometer system was that the pressure gauge was not displaying the correct pressure. The pressure inside the cell was approximately 67.4 mTorr while the pressure gauge was displaying a reading of 0.7 mTorr. To record a narrower spectral linewidth, the pressure gauge should either be calibrated to ensure accurate readings or a new pressure gauge should be purchased. Additionally, connecting a diffusion pump to the rotary vacuum pump would achieve lower pressures in the cell, contributing to a narrower linewidth and more precise spectral measurements.

In order to improve the sensitivity of the final spectrometer system, the effective optical path length of the absorption cell can be extended. Referring back to Beer's Law, as the path length increases, the interactions between molecules and the incident radiation increases, leading to higher levels of absorption. Through the use of reflectors and mirrors in the system, radiation can be reflected back through the cell to make multiple passes, increasing the effective optical path length. An additional project could include the design of a circular multi-pass absorption cell, where the geometry of the cell allows for light to be reflected in a star pattern. The number of points on the star indicates the number of beam passes and is determined by the incident angle of reflection [16].

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