

Introduction

Though chirality—the property of some molecules to be non-superimposable with their mirror image—has been known for over a century, it continues to be a focal point of research due to its real-world applications in the realm of pharmaceuticals, material development, and even quantum mechanics. While several methods have been developed to study chiral species, most require a large amount of sample to be destroyed as well as long acquisition times. However, a new chiral detection method, called microwave three wave mixing (M3WM), has the potential to solve these issues while also having great accuracy and precision [1].

Theory

The M3WM technique works by using a microwave spectrometer to obtain the phase of the free induction decay produced by the system being studied. While the signs of any two of the three dipole moments for a molecule are arbitrary, the sign of the combined quantity, $\mu_a\mu_b\mu_c$, changes with enantiomer—one of a pair of molecules produced by a chiral center [1]. If microwave radiation is used to probe transitions involving μ_a and μ_c with two orthogonal microwave fields, the phase of the molecular signal involving μ_b in the third mutually orthogonal direction differs by π radians between enantiomers [1]. This allows for the detection of enantiomers via M3WM.

Research Goals

The goals for this project were as follows:

- 1.) Design and build a microwave spectrometer capable of performing M3WM.
- 2.) Verify the spectrometer's M3WM capabilities using R- and S-carvone.
- 3.) Test the spectrometer's ability to detect both enantiomers in a racemic mix of carvone.

Instrumentation Design

The design for the M3WM spectrometer was based off the work of Schnell, Patterson [1], and Pate [2]. Unique to this instrument is the use of two arbitrary waveform generators to simultaneously generate the two desired microwave pulses needed for M3WM.

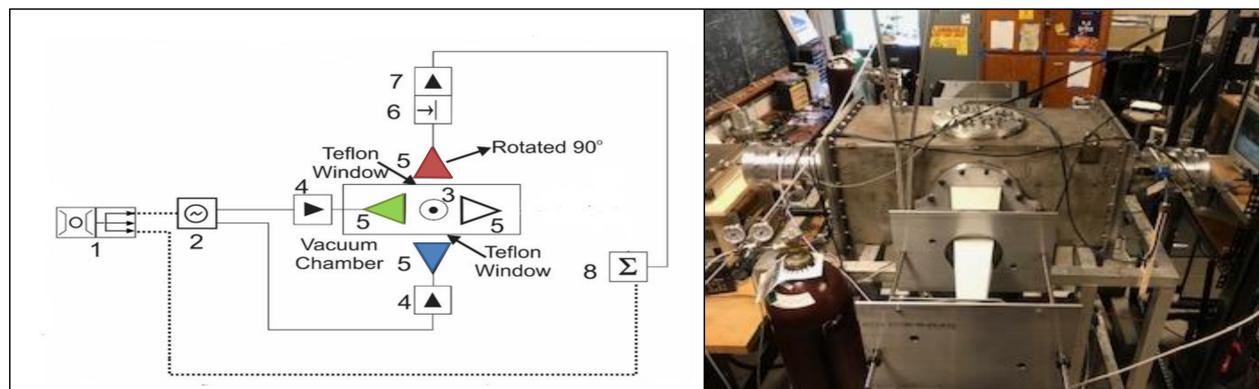


Figure 1: The M3WM spectrometer is comprised of three systems: a source for sample introduction (3), a vacuum chamber, and a circuit. Within and around the instrument are four horn antennas (5), which will be used to stimulate and detect molecular signal. The circuit—comprised of two pulse generators (2), two power amplifiers (4), a switch (6), LNA (7), and oscilloscope (8)—will be utilized to generate the microwaves and record the resulting spectra.

Methods and Verification

In order to test the capabilities of the spectrometer, the enantiomers of carvone (**Fig. 2**) were analyzed with the following mixing scheme (**Fig. 3**). First, a $\pi/2$ pulse (representing a $1/2$ population inversion in the Bloch equations) of microwave radiation was sent into the chamber via the blue horn (**Fig. 1**) at 15.8137 GHz. Immediately following, a π pulse (representing a full population inversion in the Bloch equations) was sent into the chamber via the green horn (**Fig. 1**) at 6.9344 GHz. The red horn (rotated 90° , **Fig. 1**) then listens for the resulting molecular signal at 8.8793 GHz. After collecting the resulting signal, the free induction decay recorded for each molecule can be studied to determine the phase of the resulting signal and subsequently which enantiomer was observed.

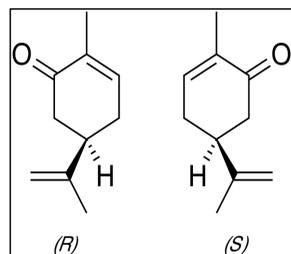


Figure 2: Enantiomers of carvone.

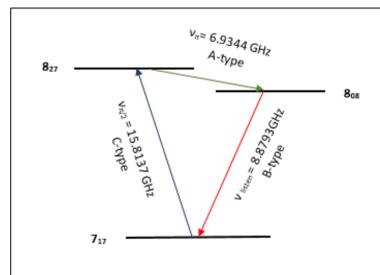


Figure 3: Mixing scheme utilized in testing.

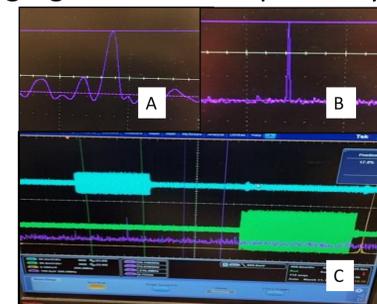


Figure 4: Timings for pulses. A.) $\pi/2$ pulse at 390 ns. B.) π pulse at 300 ns (600 ns used in scheme). C.) Resulting pulses coming from the arbitrary waveform generators.

Conclusions

As of the time of this poster submission, the timings for the $\pi/2$ and π pulses have been verified. However, the resulting molecular signal involving μ_b has yet to be observed. Some possible explanations for this are as follows:

1. While the described mixing scheme meets all for the required properties to be a viable option, it is possible that there could be some unknown energy barrier preventing the scheme from being completed. Other mixing schemes are currently being designed and tested.
2. It is possible the amplifiers used within the circuit may not be producing enough power to promote ample molecules into the desired excited states, thus resulting in the observed signal being below the spectral noise floor. Possible alternatives to the circuit are currently being investigated.
3. Finally, while the timings for the pulses appeared adequate individually, it is possible that once mixed, the timings no longer represent a true $\pi/2$ and π pulse.

References

1. Patterson, D.; Schnell, M.; Doyle, J.M. (2013) *Nature*, 467. 475
2. Lobsiger, S.; Perez, C.; Evangelisti, L.; Lehmann, K.K.; Pate, B.H. (2015). *J. Phys. Chem. Lett*, 6, 196.

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