Motivation

The goal was to gain an understanding of the reactive chemistry in the interstellar medium through the use of rotational spectroscopy to study methyl and ethyl formate.

Introduction

The main focus of the experiment was to identify trans-methyl formate in the interstellar medium. There are two conformers of methyl formate — cis- and trans — which are based upon its rotation about the C-O bond axis. For a long time, the more abundant cis conformer of methyl formate had been known to exist in the interstellar medium. Until recently, the interstellar detection of the higher energy trans-methyl formate had not been seen because its laboratory spectrum was unknown. Based on the theoretical abundances of cis and trans methyl formate, its interstellar presence would be doubtful. With a laboratory spectrum in place, Muckle et al. posed a question on the interstellar formation of trans-methyl formate. Based on two proposed theoretical pathways, it was determined that when using one reaction pathway (the Fischer Esterification), cis methyl formate was more favorable than trans; however, another possible barrierless reaction pathway (the methyl transfer reaction) helped explain the abundance of trans-methyl. Based on correlations between experimental and theoretical evidence, the GBT was used in the detection of interstellar trans-methyl formate.

Methods

Broadband Spectrometer

- Assemble various components regarding the spectrometer to run
- Adjust Necessary Controls to Desired settings
- Test Set-Up to ensure no leaks, correct pressure, and proper controls
- Run Spectrometer overnight

Theory

- Gauss fit 09
- Spartan
- QTT for calculations to find transition states
- Optimizations and frequency analysis to determine geometric optimization
- Which gives rotational constants and energies
- A 2D scan requires a special type of optimization known as the S-torsional function

Analysis

- Identify lines by comparing frequencies with those found in Spathion Database — there are known methyl derivatives of C-O and carboxylic acids for later determination
- J values used for spectral fitting

Potential Energy Surface

Theoretical calculations identify the potential energy surface and rotational constants of a molecule. The potential energy surface of a molecule is the energy of a molecule as a function of its structure. As the parameters of the molecule are adjusted, the energy levels change. In a 2-Dimensional Scan, two parameters are adjusted, such as two dihedral angles. The maximum states on these energies maps (the red areas) represent the instability at the transitional state. The minima on these maps (the blue areas) represent the stable forms called conformers. Reading along one side of a two-dimensional scan would show the change in energy if only one parameter were to change.

Reaction Pathway: Fischer Esterification

The Fischer Esterification reaction mechanism produces an acid with an ester and water. The Fischer Esterification mechanism is an energetically unfavorable reaction process. It requires energy to be put into a system to allow the reaction to occur. It is usually found in biological systems and the energy input may be controlled.

Conclusion

Based on the data, it has been confirmed that both cis and trans methyl formate are, in fact, in the interstellar medium. The cis was determined to be the more energetically favorable molecule. The spectra identified the two states, A and E, that were due to the internal rotation of the methyl group. Furthermore, it was possible to conclude that bond on results obtained in the lab, and based on comparisons in the GBT primers data, trans-methyl formate was detected in the interstellar medium. In fact, the amount of trans-methyl formate seen in the interstellar medium seems to suggest kinetic control rather than thermodynamics.

Lactic Acid and Water Clusters

In addition to the experiments that were performed on methyl formate, the spectrum is useful for a variety of other experiments. For example, a proton in the interstellar region program was also spent researching, running calculations, and performing experiments on lactic acid in efforts to help other colleagues. Pictured below is a spectrum that was collected. The microwave spectrum of lactic acid had previously been reported by van Eck. A theoretical investigation of lactic acid plus water had been performed by Smiga et al.

Finding

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