Microwave Spectroscopy of Pyridine-CS$_2$

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What is rotational spectroscopy?

- Most accurate method of determining 3D geometry of small molecules
- Provides information about molecular and electronic structure
- (Right) Structure of H$_2$SO$_4$·H$_2$O complex with the bond lengths and bond angles

Pyridine-CO$_2$

- Studied because CO$_2$ exhibits interactions with nitrogenous organic heterocycles
- Relevant as organometallic frameworks use imidazole-type linkers
- The complex has a planar structure with the nitrogen van der Waals bonding with the carbon in CO$_2$
- No internal rotations were observed and the structure below was consistent with the predicted geometry

Molecular Axis System

- The a-b-c axes are principle axes for the inertial tensor and are the natural axes to described the rotation of a molecule.
- Rotational transitions occur when the molecular dipole moment interacts with the electric field of radiation.
- Dipole moment projects onto a, b, c axes as $\mu_a$, $\mu_b$, and $\mu_c$.
- Depending on the interaction, different selection rules for rotational transitions are employed.
- Molecules can have a mix of a, b and c transitions as seen below.

Pulsed-Nozzle Fourier Transform Microwave Spectroscopy (FTMW)

[Diagram of experimental setup]

Nozzle Assembly

Our nozzle assembly utilizes a supersonic jet expansion in conjunction with a laser ablation target, allowing us to cool ablated molecules to low-lying energy levels, thus simplifying our observed spectra.

CO$_2$ & CS$_2$ Comparison

- Similarities:
  - Do not have an overall dipole moment
  - Have group VI elements complimenting carbon
- Differences:
  - Have opposite quadrupole moments

Why Pyridine-CS$_2$?

- Since the sign on the quadrupole moment is opposite from that of carbon dioxide, we are interested in observing whether this is the dominating effect on the change of structure of the complex.

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