Microwave Spectroscopy of Pyridine-CS_2

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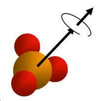
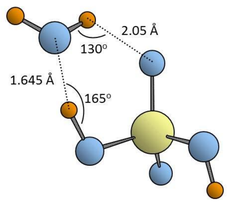
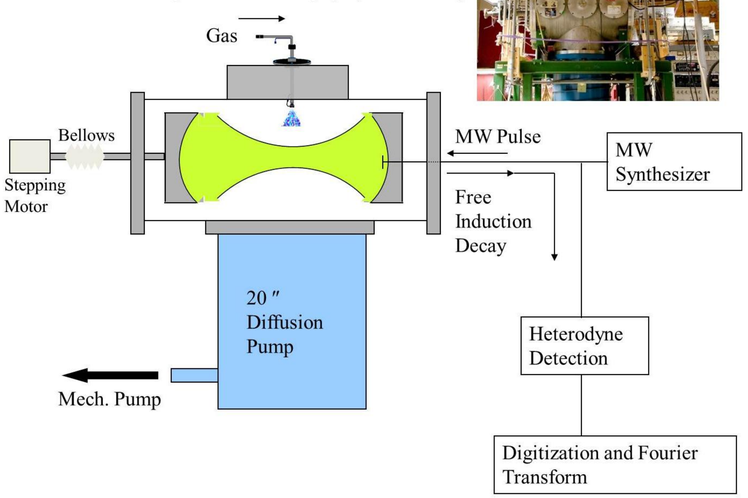
What is rotational spectroscopy?

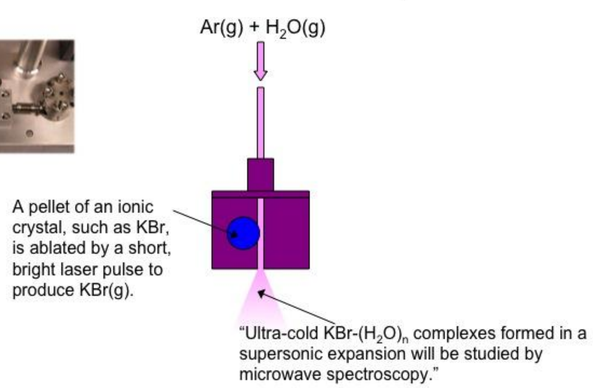
- Most accurate method of determining 3D geometry of small molecules
- Provides information about molecular and electronic structure
- (Right) Structure of H_2SO_4-H_2O complex with the bond lengths and bond angles





Pulsed-Nozzle Fourier Transform Microwave Spectroscopy (FTMW)



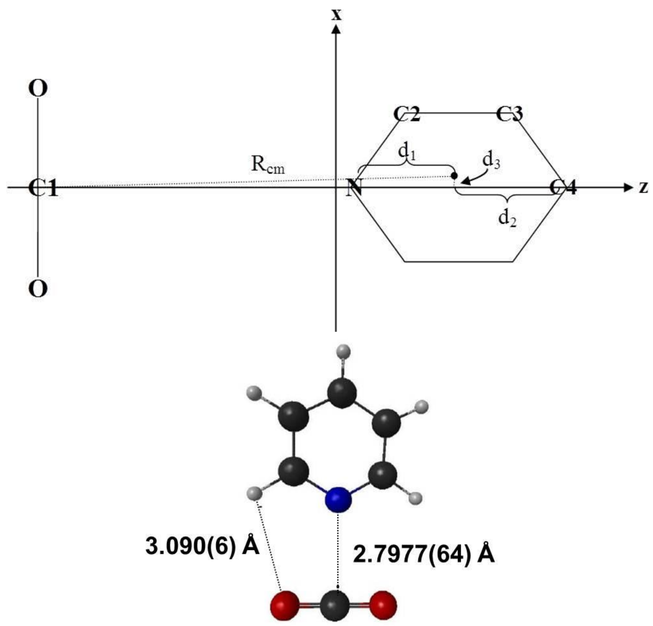


Nozzle Assembly

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.

Pyridine-CO_2

- Studied because CO_2 exhibits interactions with nitrogenous organic heterocycles
- Relevant as organometallic frameworks use imidazolate-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



CO_2 & CS_2 Comparison

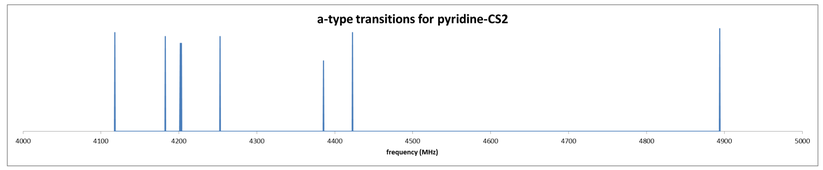
- Similarities:
  - Do not have an overall dipole moment
  - Have group VI elements complimenting carbon
- Differences:
  - Have opposite quadrupole moments

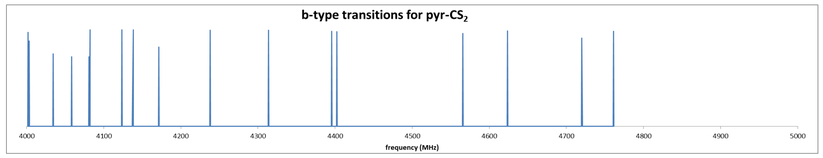
Why Pyridine-CS_2?

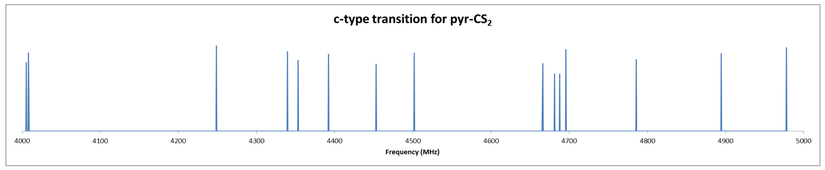
- Since the sign on the quadrupole moment is opposite from that of carbon dioxide, we are interested in observing whether this is the dominating effect on the change of structure of the complex.

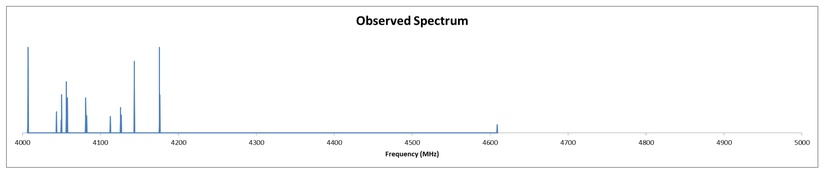
Molecular Axis System

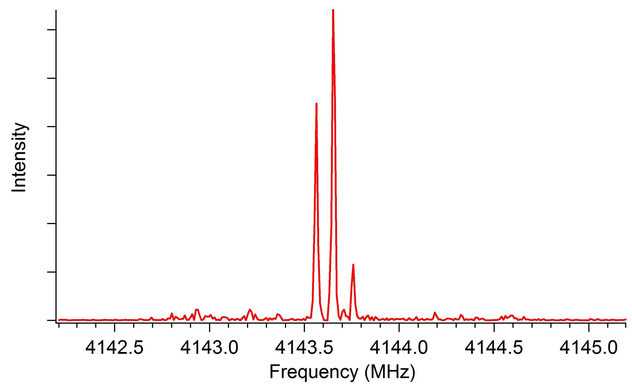
- The a-b-c axes are principle axes for the inertial tensor and are the natural axes to described the rotation of a molecule.
- Rotational transitions occur when the molecular dipole moment interacts with the electric field of radiation.
- Dipole moment projects onto a, b, c axes as μ_a, μ_b and μ_c.
- 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.











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