School of Natural and Environmental Sciences

Microwave Spectroscopy: Imidazoles

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Aims

- **Collect spectra for Imidazole derivatives (4-(5)-methylimidazole)**
- **Analyse the spectra using Western's Pgopher[1] software**
- **Obtain rotational, centrifugal distortion and nuclear quadrupole coupling constants in order to help elucidate the structure of these molecules in the gas phase**

Introduction

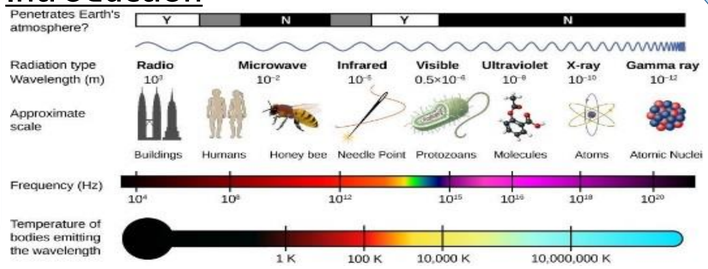

Fig.1 – The Electromagnetic Spectrum (www.phys.libretexts.org)

- Microwave spectroscopy is a tool used in molecular structure determination, particularly investigating weak interactions such as hydrogen bonding and Van Der Walls forces by probing rotational motion in molecules.
- A permanent dipole moment (polarity) is required to polarise transitions and probe molecules, producing the spectra we observe.
- Understanding how biological molecules interact together, with water and with other molecules is of great interest. Imidazole is found in many biological compounds, hence, Imidazole derivatives tend to have important medicinal properties.

Carbon Monoxide: An example

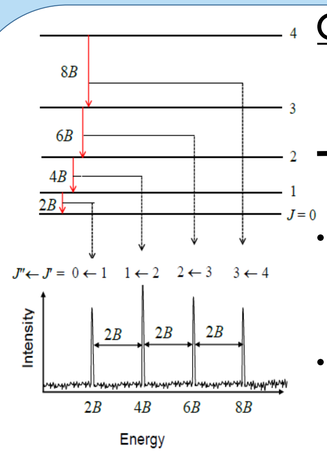

Fig.2 – Energy levels and spectral line positions that are specific to a linear diatomic molecule. (www.wikipedia.org, date accessed: 14/08/18)

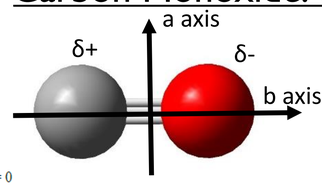

Fig.3 – Red = Oxygen, Grey = Carbon. Labelled are the internal axes of rotation of a CO molecule. There is a c axis coming in and out of the page where the b and a axes meet. A dipole moment exists coaxial to the a axis.

- Molecules in the gas phase rotate around a set of mutually perpendicular axes with fixed orientation in space dependant upon the mass of the molecule.
- Rotation about these axes are linked with a set of specific energy levels dependant upon moments of inertia (torque needed for angular acceleration about a rotational axis).
- Spectroscopic analysis of molecules produces a quantitative result linked to the moments of inertia. From this, values for the structure of molecules can be elucidated. Molecules can tend to be much more complicated than CO however…

4-(5)-methylimidazole

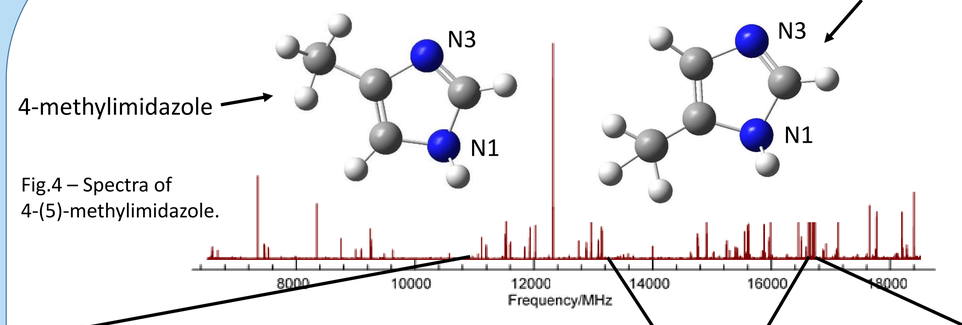

Fig.4 – Spectra of 4-(5)-methylimidazole.

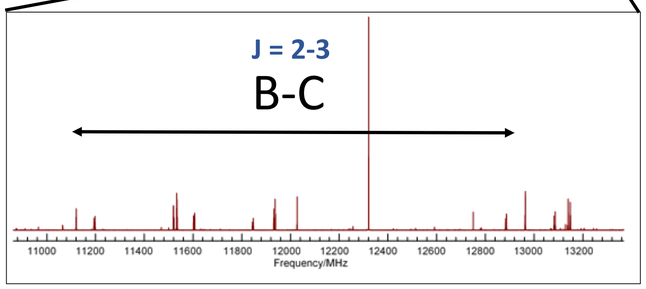

Fig.5 – Expanded in section of 4-(5)-methylimidazole spectra. J = Total angular momentum quantum number.

- The arrow above indicates the width of an A-type transition B-C = 1850 MHz using pgopher[1].
- This is a large value meaning the molecule is oblate (Frisbee like shape) rather than prolate (rugby ball).

Results and Experimental

- A bespoke Chirped Pulse Fourier Transform Microwave (CP-FTMW) spectrometer was used for the experiments.
- Measurement of spectra in the 6.5 – 18.5 GHz range.
- A pulsed ND:YAG laser was used to vaporise the materials under study into the gas phase in the presence of an Argon atmosphere at 2 K.
- Recently, the laser was altered to the fundamental wavelength (1064nm). This was shown to produce a better signal to noise ratio with the Organic molecules currently under study compared to the previous 532nm double frequency setting.

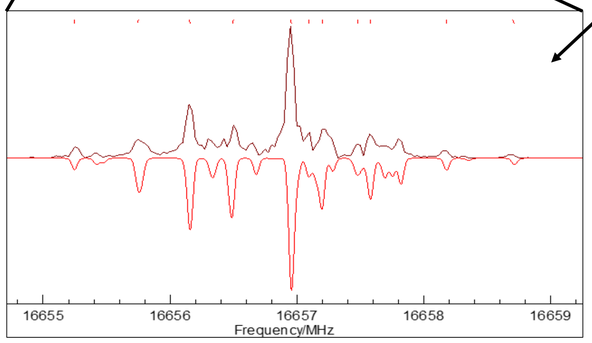

Fig.6 – Expanded section of 4-(5)-methylimidazole spectra showing a 4-methylimidazole transition.

- 4-methylimidazole observed spectra and analysed spectra (inverted) using Western's pgopher[1].
- Splitting from the two quadrupolar Nitrogen nuclei, spin quantum number I > ½ .
- Quadrupolar nuclei have an asymmetric charge distribution. An electric field gradient (electrons in the sample) can exhibit a torque on the nucleus creating a quadrupole moment. This allows for spectra to be collected.

Imidazole

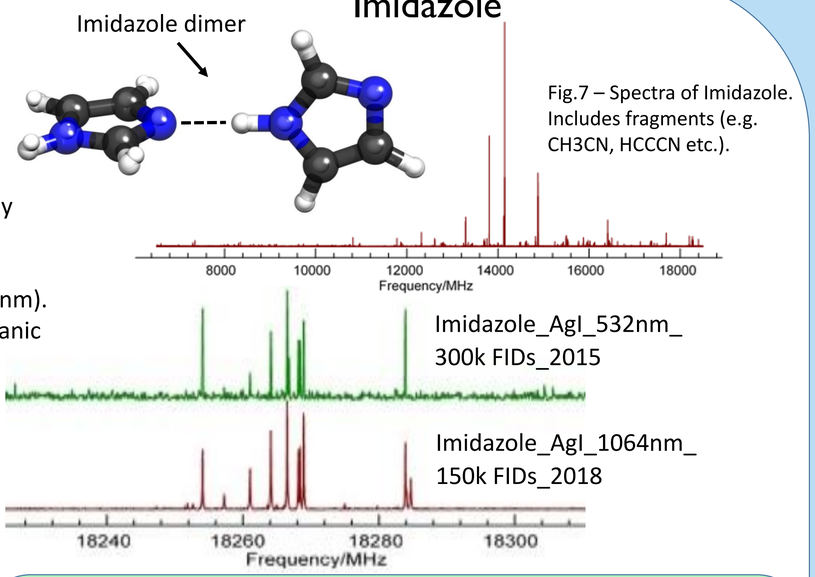

Fig.7 – Spectra of Imidazole. Includes fragments (e.g. CH3CN, HCCCN etc.).

Conclusion

- **Spectra for 4-(5)-methylimidazole was obtained and analysed using Western's pgopher[1]**
- **Rotational constants, centrifugal distortion and quadrupole coupling constants were deciphered for 4-(5)-methylimidazole**
- **For future work, determining how the molecules interact and complex with water (where does the H_2O molecule hydrogen bond to?)**

1. Western's Pgopher, http://pgopher.chm.bris.ac.uk/, (date accessed: 24/08/18)