# SPECTROSCOPY

From the word

***Spectre***

ˈspɛktə Noun Latin
A visual apparition.
– ghost.

and

***Spec-trum***

ˈspɛktrəm Noun
A characteristic series or range, used to classify something on a scale, often referring to colours.

***Scope***

skəʊp Noun Spanish
Instrument used for viewing spectra.
Originally associated with Spanish rifles.

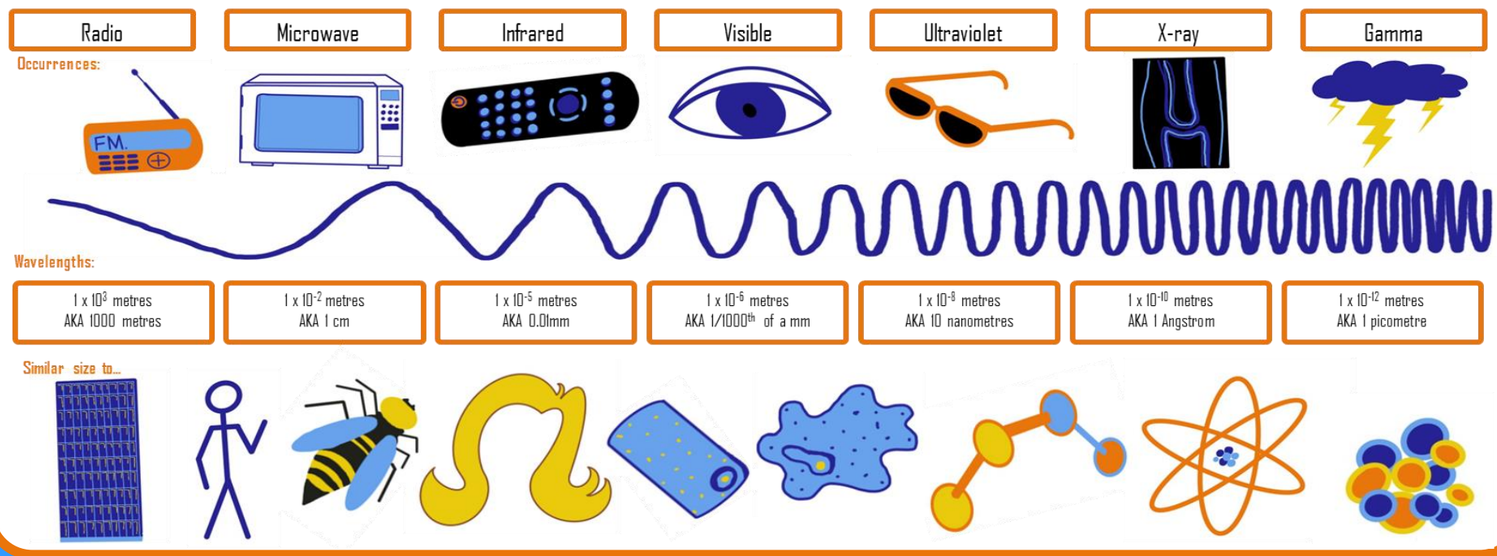
and the suffix

***Skopion***

skɔːpiən Verb Greek
To observe, examine or study.
Also Scorpion.

## The Electromagnetic Spectrum

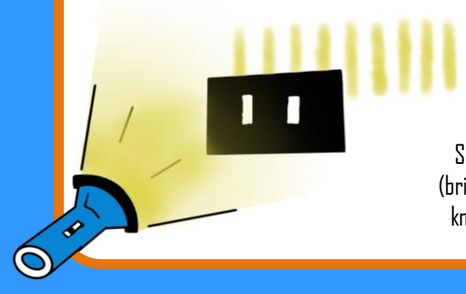
Electromagnetic (EM) waves travel all at the speed of light when in a vacuum (approximately 300million metres per second), and slower when passing through matter. Different types of radiation arise from different frequencies of EM waves, including visible light. Below are some examples of EM waves, their relative sizes and some uses.




## Light

The word 'spectroscopie' was first used over 100 years ago. Nowadays, spectroscopy describes the scientific discipline of studying how light –EM radiation – interacts with matter. Conversely, spectro**metry** describes the process of measuring these interactions and often will apply to analytical techniques that do not use light.

Light has the interesting ability to be studied in multiple ways. The physics concept known as **Wave-Particle Duality** shows how light can be described as a particle; a **photon** with associated **energy**, and as a **wave**: with various **frequencies**.



This is a modern demonstration of **Young's Double Slit Experiment** (originally performed in 1801) showing an example of how light can behave as a wave.

Some of the waves pass through the gaps and combine (bright section) and some cancel out (the shadows). This is known as **constructive and destructive interference**.

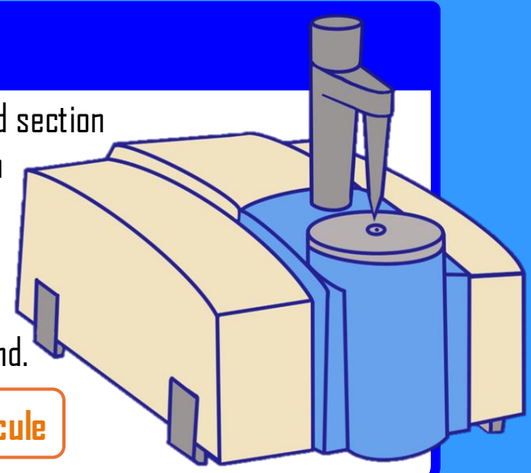
## Infrared Spectroscopy

**History:** Originally described as 'radiant heat', William Hershel noticed an unusual spike in temperature after attempting to measure the temperature of the red section of visible light, marking the first observation of Infrared (IR) frequencies in 1800. The frequency of IR waves are between **300 Billion-430 Trillion Hertz** with a wavelength similar size to that of a needle-point or a human hair.

**Theory**: Bonds **vibrate** in many different ways when a molecule is at a temperature above absolute zero. When an IR frequency matches the natural vibrating frequency of a bond, the **energy** is absorbed, and the amplitude of the vibration is increased. Different types of bonds have different vibrations. These are measured using the **wavenumber cm$^{-1}$**, which is the **inverse** of the **wavelength** and therefore **proportional** to the **energy** and **frequency** of the vibrating bond.

**Applications:** Quality control, breathalysers, drug safety testing, art restoration.

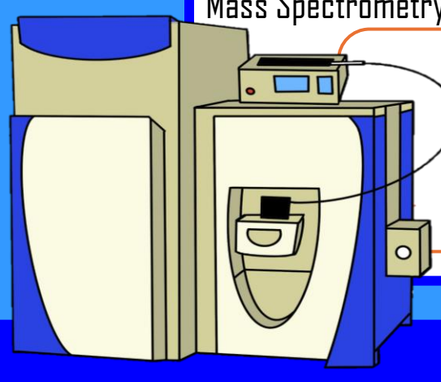
**AIM: Identify Functional Groups and bond types within a molecule**



Mass Spec is over 1000 x more sensitive than IR!

## Mass Spectrometry

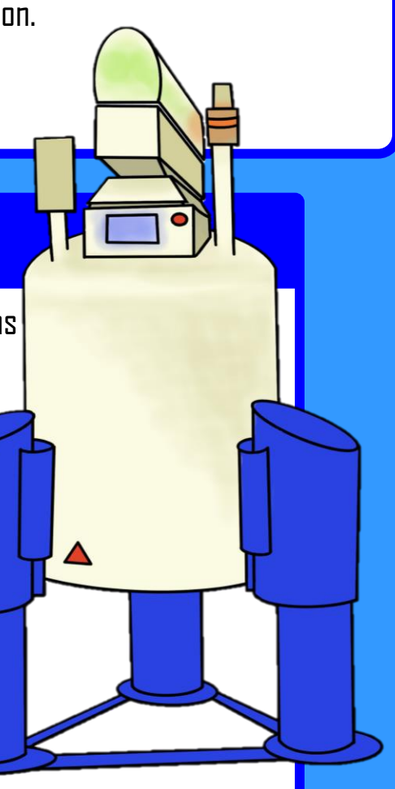
Mass Spectrometry does not use the EM spectrum, hence not being called a spectro**scopic** technique. It does, however, utilise the effects an **EM field** has on ions.



**AIM: Determine the connectivity of a structure by identifying fragments**

**Theory:** Any flow of charge (**electrical current**) from electrons (or positively charged ions) has an associated **magnetic field**. This **EM field** will deflect when put into an external magnetic field and travel forwards. A Mass Spectrometer breaks a sample into ions to exploit this physics in the following process: 1. Vaporisation. 2. Ionisation. 3. Acceleration. 4. Deflection. 5. Detection.
**Heavier** ions travel **slower** and hit the detector after the **lighter**, **smaller**, **quicker** ions.

**Applications:** Airport security, pharmacology, astrology, athletic drug testing.



## Nuclear Magnetic Resonance

**Theory**: **Protons** and **Neutrons** each have '**spin**', just like the needle on a compass, aligning with the geomagnetic field of Earth. The magnetic spin of protons and neutrons align with an external EM field. If a molecule has an **even** number of protons and neutrons these spins cancel out to zero. But with an **odd** number, like $C^{13}$ or $H^{1}$, the atoms have a magnetic moment. A sample is placed within a liquid helium-cooled **EM field**. This causes the atoms with a **magnetic moment** to **align** with the field in a relaxed state. **Radio waves** are applied and absorbed by the atoms, lifting them to an **excited state**, in opposite spin to the field (**resonance**). As the atoms relax back to the aligned spin state, energy is **emitted.** NMR spectrometers measure the resonance and produce a spectra, plotting the different atomic environments' **shift** in **parts per million** (ppm). This 'shift' refers to a comparison to a standardised measurement, often tetramethylsilane (**TMS**), which is set to zero.

**Applications**: MRI body scans, environmental monitoring, quantum computing.

For Proton NMR try remember the following:
Number of peaks = The number of different hydrogen environments/positions.
**Integration** of a peak = The number of hydrogens in that environment (a ratio).
Position of a peak (**chemical shift**) = The type of functional group/s.
The **splitting** of a peak = The number of hydrogens in neighbouring environments. This uses the **n+1 rule**.

**AIM: Locate the positions/environments of atoms in a molecule by identifying the functional groups and connectivity.**




## WHERE COULD SPECTROSCOPY TAKE YOU?

You've seen how Spectroscopy can be used in many different instruments, these are only some of the most common examples. But all of these techniques are used in many different fields of study – many never even entering a laboratory! Analytical chemistry is one of the broadest fields of research and can lead into so many different careers.

Chemistry courses at Universities can almost always be modified to suit your best and favourite topics so that you can make the most out of your degree and the skills that you've learnt. University isn't the only way to get a career or a degree. Apprenticeships are becoming more popular and can allow you to gain a degree, qualifications and a paying job all at the same time!

Thank You for taking part in the **Spectroscopy in a Suitcase Workshop** from The University of Southampton.