ENGINEERING CHEMISTRY

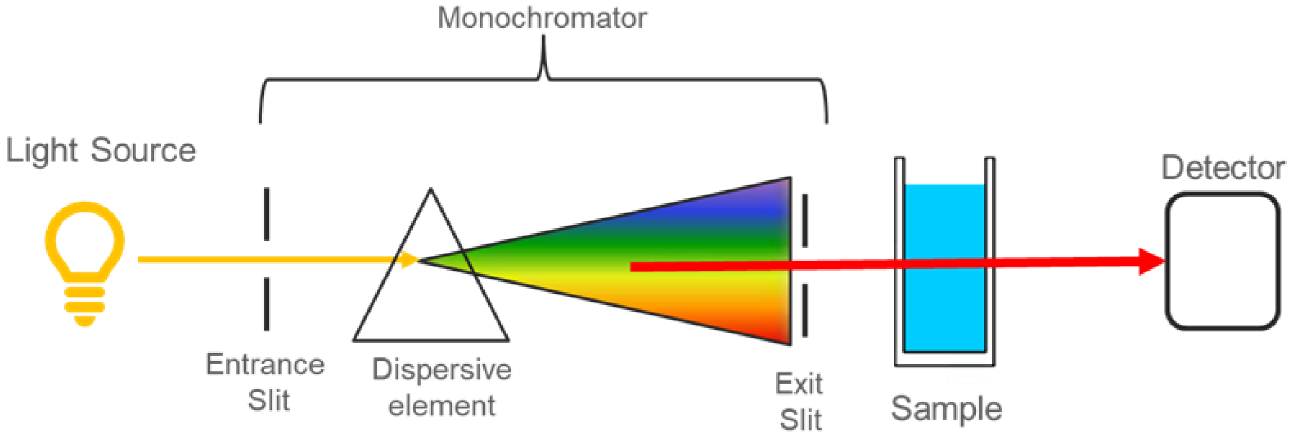
Department of Science and Humanities

- ***Interaction of electromagnetic radiation with matter***
- ***Electromagnetic spectrum***
- ***Born –Oppenheimer approximation***
- ***Microwave spectroscopy- diatomic rigid rotor model and the rotational spectrum***
- ***IR spectroscopy- diatomic harmonic oscillator and anharmonic oscillator model***
- ***Electronic spectroscopy- Vibrational coarse structure(Progressions), Franck Condon Principle***

Class content :

- ***Definition of Molecular spectroscopy***
- ***Interaction of electromagnetic radiation with matter***
- ***Comparison between atomic and molecular spectra***
- ***Quantisation of energy***
- ***Absorption and emission spectra***
- ***Spectroscopic units***

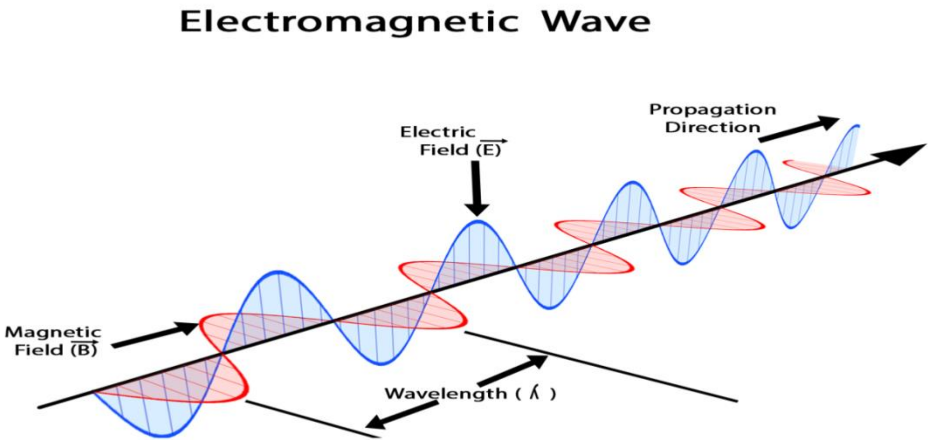
- **Molecular spectroscopy** is that branch of science which deals with the study of **interaction of electromagnetic radiation with matter(molecules)**
- **Incident radiation → diffraction grating → sample → detector→ recorder**(spectrum)



UV Vis Spectroscopy (https://www.smacgigworld.com/)

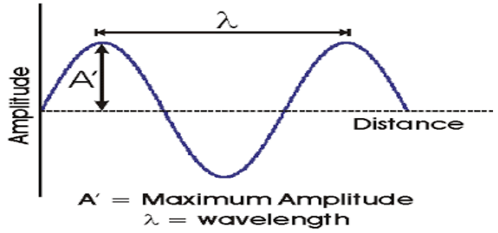
Some important features of **electromagnetic radiations** are:

- They have **dual character** i.e. particle character as well as wave character, for example, a beam of light is a stream of particles called photons moving through the space in the form of waves
- These waves are associated with **electric and magnetic fields** oscillating perpendicular to each other and also perpendicular to the direction of propagation
- All electromagnetic radiations travel with the **velocity of light**



Source:https://byjus.com/physics/characteristics-of-em-waves/

Waves can be characterised by the following **properties** :



http://www.chemistry.wustl.edu/~coursedev/Online%20tutorials/Waves.htm

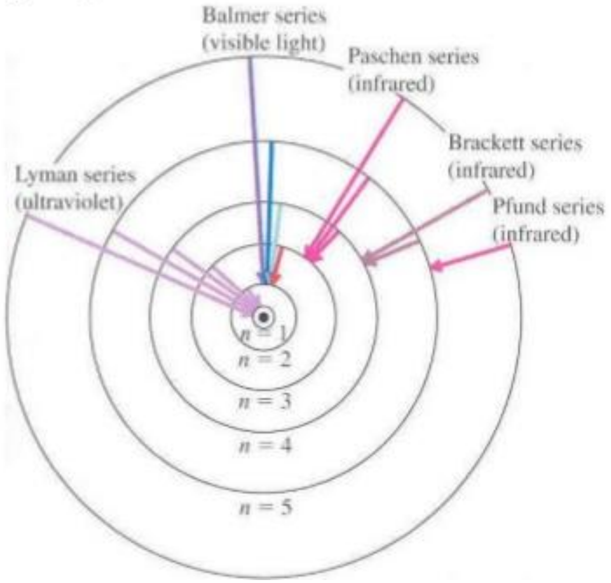
- **Wavelength** : The distance between two successive crests and troughs of the wave ; **λ** ; m , nm or Å
- **Frequency** : The number of cycles completed in a certain amount of time ; **ν** ;Hz or s^{-1}
- **Wave number** : Number of complete waves or cycles contained in unit distance ; $\bar{\nu}$, cm^{-1}
- **Energy** of electromagnetic radiation is given by **E= hν** , where E is energy, h is Planck's constant,(h= 6.625 x 10^{-34} Js), and ν is frequency
- Wavelength is related to frequency by **ν = c/λ** , where c is the speed of light, λ is wavelength, and ν is frequency
- Wave number is related to wavelength by

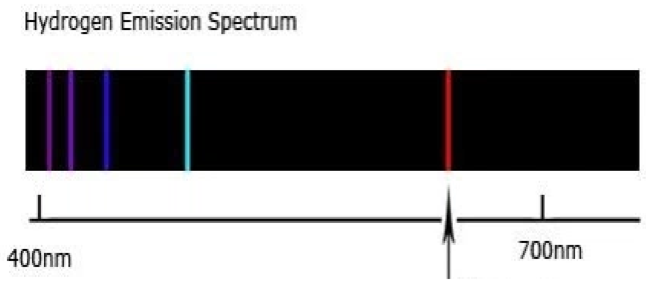
$$\bar{\nu} = \frac{1}{\lambda}$$

Comparison between atomic spectra and molecular spectra

Atomic spectra

- Due to electronic transitions from **one atomic orbital to another**
- Gives rise to **line spectra**



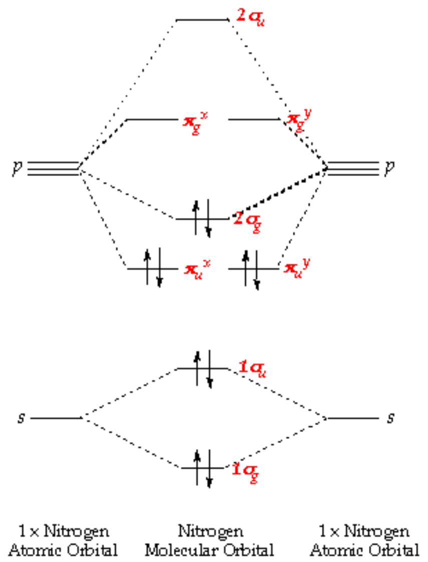


Source:https://socratic.org/questions/what-happens-to-the-distance-between-energy-levels-at-higher-energy-levels

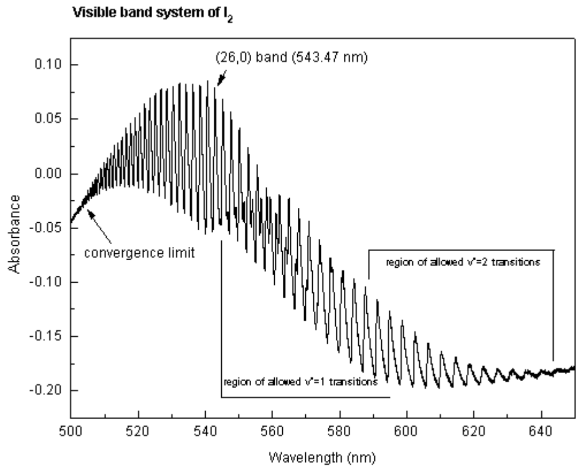
Source:https://www.slideshare.net/mizakamaruzzaman/phy-310-chapter-5

Molecular spectra

- Due to electronic transitions from the **Highest occupied molecular orbital**(HOMO) to **Lowest unoccupied molecular orbital**(LUMO)
- Gives rise to **band spectra** due to rotational and vibrational transitions possible in molecules along with electronic transitions



Source:https://socratic.org/questions/what-are-the-molecular-orbital-configurations-for-n-2-n-2-2-n-2-n-2-and-n-2-2



Source:https://chem.libretexts.org/Courses/Pacific_Union_College/Quantum_Chemistry/13%3A_Molecular_Spectroscopy/13.06%3A_Electronic_Spectra_Contain_Electronic%2C_Vibrational%2C_and_Rotational_Information

Quantisation of energy

- Energy levels in atoms or molecules are discrete or **quantised**
- Energy can be absorbed only in packets called **quanta**
- Frequency of light absorbed when there is a transition between two energy levels depends on the **difference in energy** between the two energy levels
- If an atom or molecule in ground state absorbs energy there exists a higher energy level corresponding to the frequency of light absorbed

E_2

$$\Delta E = E_2 - E_1 = h\nu$$

E_1

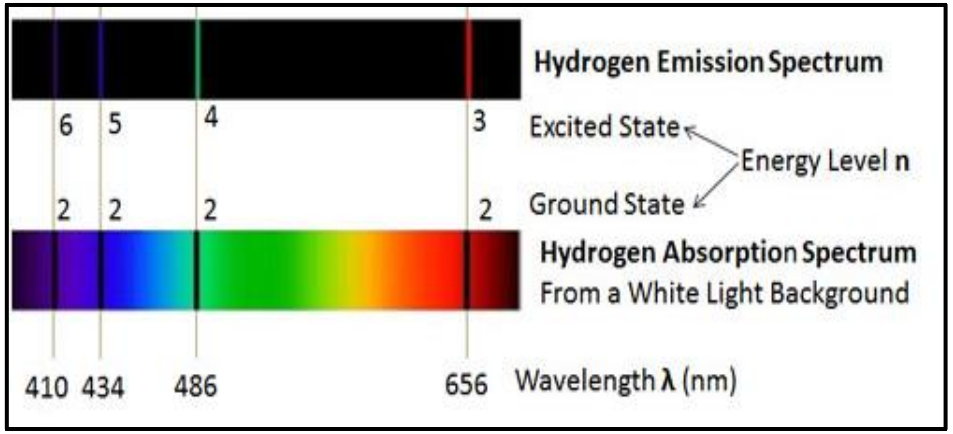
Absorption and Emission spectrum

- **Absorption spectrum** is observed when an atom or molecule absorbs energy and moves from lower energy level to higher energy level
- **Emission spectrum** arises when molecule comes from higher energy level to lower energy level

$$\Delta E = E_2 - E_1 = h\nu$$

E_2

E_1



Spectroscopic units

$E=h\nu$ where Energy is expressed in Joules

Wave number is related to wavelength by $\bar{\nu} = \frac{1}{\lambda}$

since $c = \lambda\nu$, $\bar{\nu} = \frac{\nu}{c}$

Therefore $E = hc\bar{\nu}$ or $\bar{\nu} = \frac{E}{hc}$

- The **spectroscopic unit** for energy of a radiation is **cm^{-1}**
- It is **energy expressed in wave numbers**
- It is for **convenience** of using small numerals

e.g. $1\ cm^{-1} = 1.99 \times 10^{-23}$ J

THANK YOU

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