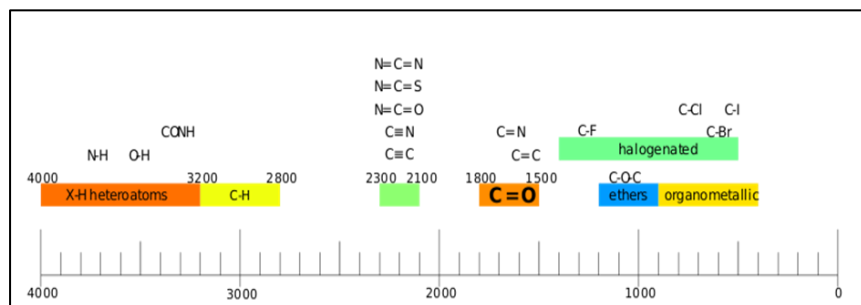
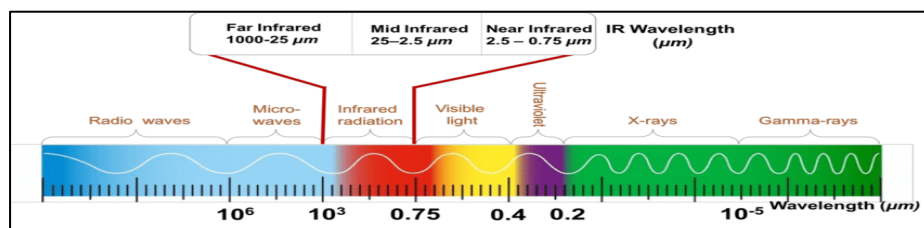


INFRARED SPECTROSCOPY

Introduction :- Infrared spectrum radiation ranges from 3000 to 30 cm wavenumber and wavelength of 0.75 to 300 μ . It lies between visible and microwave region in the electromagnetic spectrum. They are formed due to changes in vibrational energy along with rotational energy. Infrared region be categorized into three distinct zones based on their wavenumbers and wavelength.



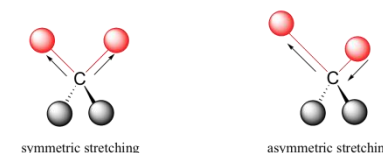
IR Spectrum



Region of IR Spectrum

Modes Of Vibration In Polyatomic Molecule

Stretching Vibration :- In this the distance between the two atoms increases or decreases but the atom remain in same bond axis. This vibration type corresponds to one dimensional motion i.e. it will have (n-1) stretching for non-cyclic system. Bond angle change only if required to do so by centre gravity resisting displacement.

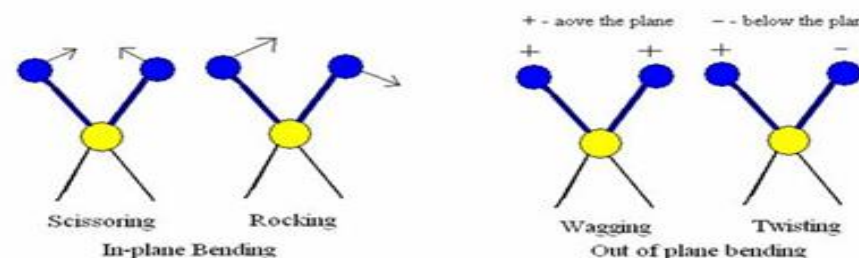


Symmetrical Stretching :-



Asymmetrical Stretching :-

Bending or Deformation Vibration :- In this there occur change in bond angle between atoms. In the three atom system it forms part of large molecule and vibration involve oscillation of atoms or group as a whole which is perpendicular to the chemical bond. It takes place in-plane or out-plane.



In-plane bending i) Symmetric ii) Rocking In symmetrical two atoms connected to central atom either move toward or away from each other with certain deformation of valence angle. In rocking structural unit swings back and forth in plane of molecules.

Out-plane bending i) Wagging ii) Twisting

Wagging occurs when structural unit swings back and forth outside plane of molecule.

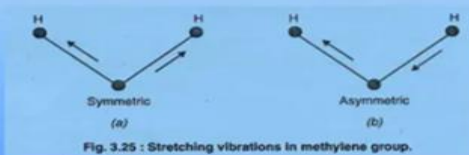
Twisting occurs when structural unit rotate about bond that joins to the rest of the molecule.

Factors Affecting Vibrations

- i) Vibrational Coupling
- ii) Hydrogen, Bonding
- iii) Electronic Effect
- iv) Field Effect

Coupling vibrations

- An isolated C-H bond has only one stretching vibrational frequency where as methylene group shows two stretching vibrations, symmetrical and asymmetrical.
- Asymmetric vibrations always occur at higher frequencies or wavenumbers than symmetric stretching vibrations. These are known as coupled vibrations.

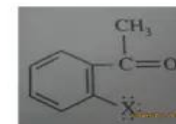


Hydrogen bonding

- Stronger the hydrogen bonding, greater is the absorption shift towards lower wave number than the normal value.
- Intermolecular hydrogen bonds give rise to broad bands and intramolecular hydrogen bonds are sharp and well defined.
- Intermolecular hydrogen bonds are concentration dependent on dilution, the intensities of such bands decrease and finally disappear. Intramolecular hydrogen bonds are independent of concentration.
- The N-H stretching frequencies of amines are also affected by hydrogen bonding as that of the hydroxyl group but frequency shifts for amines are lesser than that for hydroxyl compounds.
- Because nitrogen is less electronegative than oxygen so the hydrogen bonding in amines is weaker than that in hydroxy compounds.

Field effect :

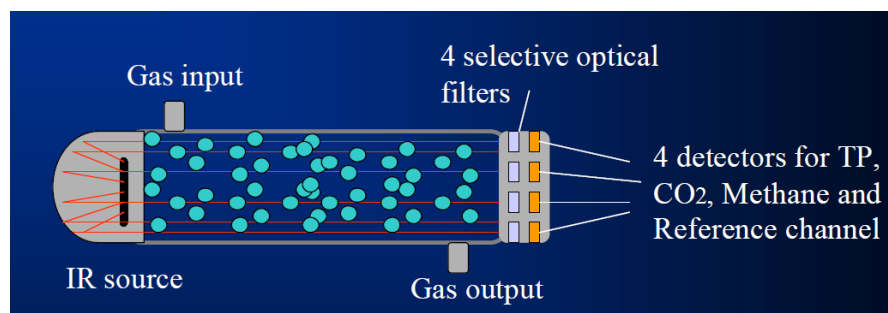
- In ortho substituted compounds, the lone pair of electrons on two atoms influence each other through space interactions and change the vibrational frequencies of both the groups.
- This effect is called field effect.



Ortho halo acetophenone

Sample Handling :-

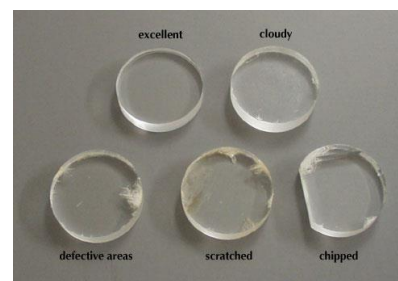
Gas : Path length used in 10 cm If this is short spectra of minor components or substance are encountered with variable path cell provide Material used for folding are gold surfaced mirror or gold plated or stainless steel metal component



Liquids And Solutions :- Samples that is liquid at room temperature are scanned in neat original form in solution Transparent region is selected to obtain spectra of polar materials. Solvents used should be susceptible to hydrogen bonding.

Films :- Capillary films are used. A large drop of neat liquid is placed between two infrared transmitting windows which are then squeezed together and mounted in the spectrometer

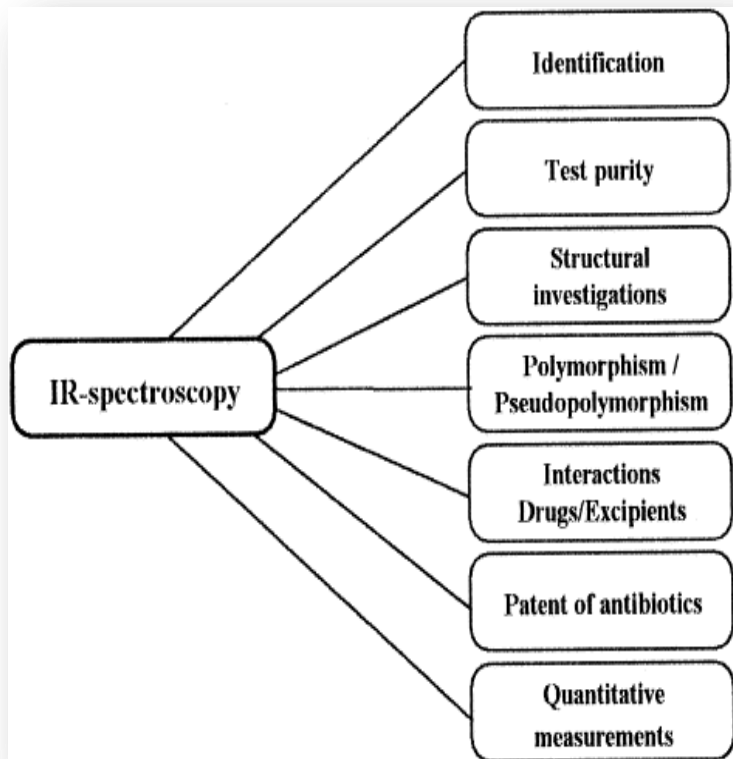
Mulls :- Sample is grounded into fine particle anal then the mulling agent in small but sufficient quantity is added. Mixture is then transferred to mull plates that are squeezed to adjust the sample



Potassium bromide (KBr):-



Application



Reference: Instrumental method of Analysis - Gurdeep R. Chatwal, Sham, A. Anand, Page no. 213 to 221.

Pharmaceutical Analysis, volume II - Dr. A. V. Kasture, Dr. K. R. Mahadik, Dr. S. A. Wadodkar, Dr. H. N. More, Nirali Prakashan Page No. 240 to 250

Instrumental methods of analysis of seventh edition willard, Merritt, Dean Settle Page no. 293 to 364

Prepared By : Uma D. Sangle

Mentor : Mrs. Asmita V. Gaikwad

Department : Pharmaceutical Chemistry

Subject : Instrumental Method Of Analysis

Class : Final Year B. Pharmacy

Acedemic Year : 2021- 2022

