STANDARD OPERATION PROCEDURE OF FTIR

NAME OF THE INSTRUMENT0 : FOURIER TRANSFORM INFRARED RADIATION (FTIR)

Name of Manufacturer : **Bruker**

Version : Alpha ECO -ATR

A. AIM: To demonstrate the standard operating procedure of Fourier Transform Infrared Radiation (FTIR)

B. OBJECTIVES:

1. To determine the types of functional groups present in the Organic substance.
2. To determine the structure of an unknown Natural/Synthetic compound.
3. To perform the qualitative analysis of substances.
4. To perform the quantitative estimation of an Organic substance.
5. To characterize and interpret the data for the evaluation of structure.

C. PRINCIPLE:

- The absorption of Infra-red radiations causes an excitation of molecule from a lower to the higher vibrational level. We know that each vibrational level is associated with a number of closely spaced rotational levels.
- The Infra-red spectra are considered as vibrational-rotational spectra. All bonds in a molecule are not capable of absorbing infra-red energy but only those bonds which are accompanied by a change in dipole moment will absorb in the infra-red region.
- Such vibrational transitions which are accompanied by a change in the dipole-moment of the molecule are called infra-red region.
- On the other hand, the vibrational transitions which are not accompanied by a change in dipole-moment of the molecule are not directly observed and these are Infra-red inactive.

Types of Vibrations:

1. **Stretching.** In this type of vibrations, the distance between the two atoms increases or decreases but the atom remains in the same bond axis.
2. **Bending.** In this type of vibrations, the positions of the atoms change with respect to the original bond axis.

The various stretching and bending vibrations of a bond occur at certain quantised frequencies.

Types of stretching vibrations:

There are two types of stretching vibrations:

Symmetric stretching: In this type, the movement of the atoms with respect to a particular atom in a molecule is in the same direction.

Asymmetric stretching: In these vibrations, one atom approaches the central atom while the other departs from it.

Types of bending vibrations: (Deformations).

Bending vibrations are of four types:

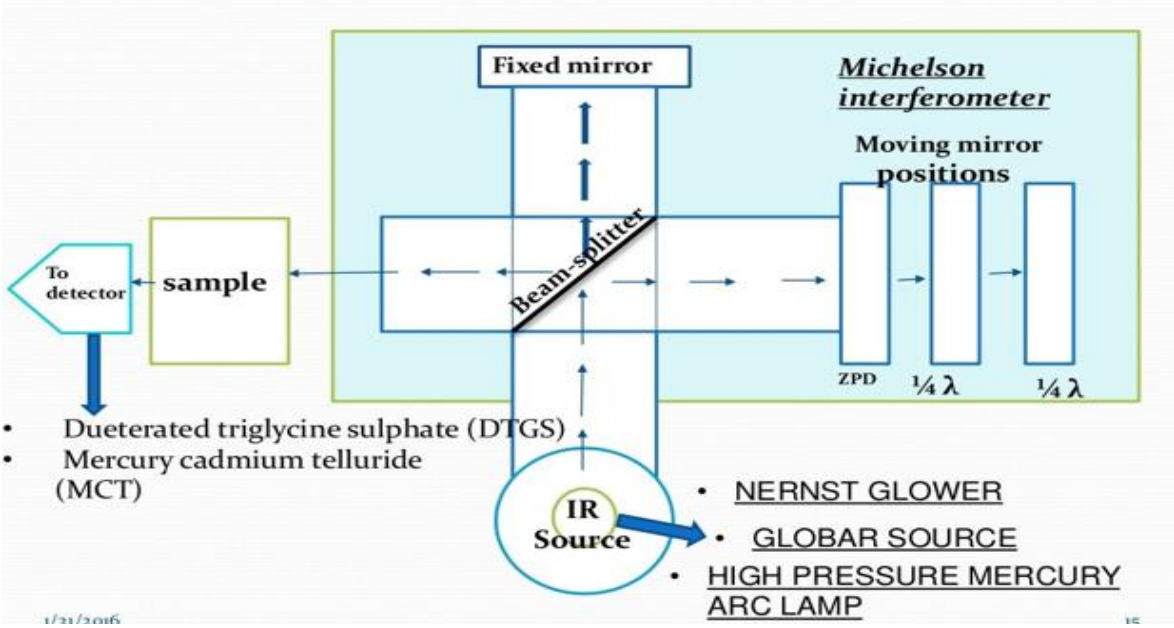
Scissoring: In this type, two-atoms approach each other.

Rocking: In this type, the movement of the atoms takes place in the same direction.

Wagging: Two atoms move 'up and down' the plane with respect to the central atom.

Twisting: In this type, one of the atoms moves up the plane while the other moves down the plane with respect to the central atom.

D. SCHEMATIC DIAGRAM:



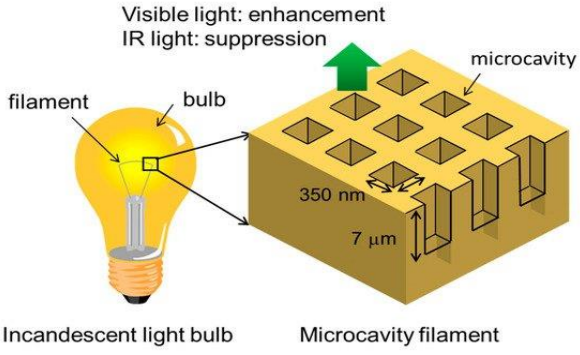
E. STANDARD OPERATING SYSTEM:

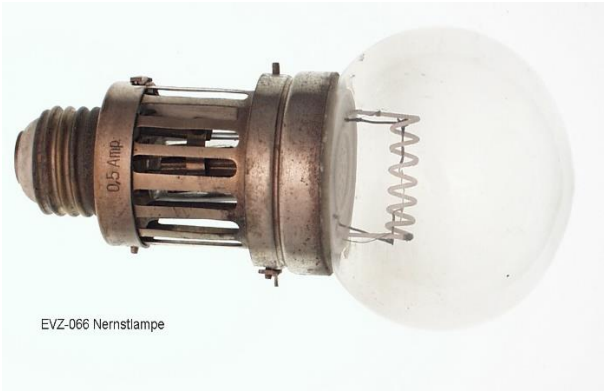
1. Switch ON PC and printer.
2. Remove sample if any and Switch ON Alpha FTIR and wait for 10 minutes. (For source warm up). After 10 minutes of warm up time LED on the Spectrometer will turn to full green, now open OPUS Software and it prompts for Password.
3. Enter Password and Click Login.
4. Software will display license Information, click on OK.

5. Select Experiment file (Go to Measurement click down arrow Select Setup Measurement select Load and load Transmission. XPM Experiment then click save & Exit).
6. Enter Sample Name & Batch No.
7. Now without keeping any sample collect Back Ground and place the sample then Click Collect Sample Spectrum.
8. Click Measurement Button, software prompts to enter Sample Name and Sample Form (Batch. No)
9. Now collected spectrum will be displayed on the Screen.
10. Now go to Peak Picking to annotate peak Labels (Drag the cursor up to required level and click Store.
11. Now take printout by clicking Quick Print.
12. To overlay two spectrums First Load Two Spectrums (Sample & Standard) to the Window, and adjust distance between two spectrums by right clicking mouse and select Shift Whole curve then drag any of the spectrum to differentiate both the spectrums and then click Quick Print.

F. FTIR COMPONENTS:

1.Radiation source

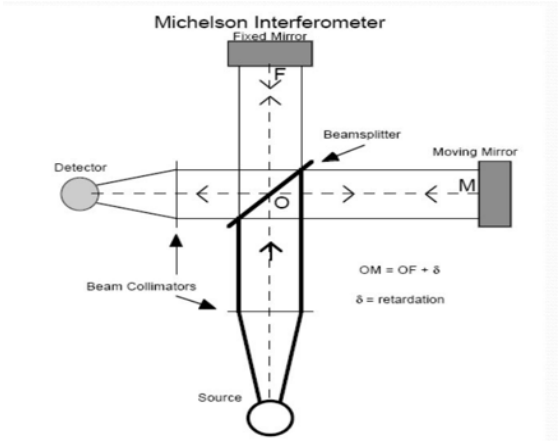




Incandescent light **Nernst glower**

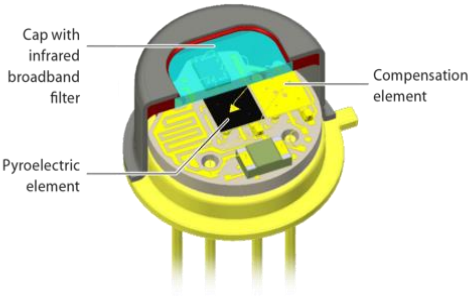
High pressure mercury arc

2. Interferometer



Michelson interferometer

3. Detector



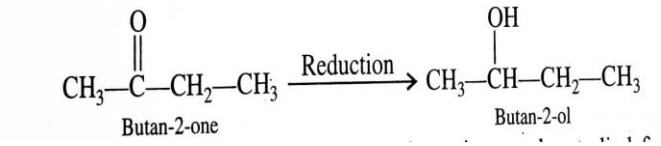
Polyelectric detector

G. SAFETY INFORMATION:

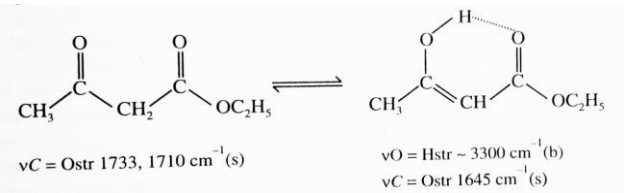
1. When using the EGA-TGA Cell remember that it is hot. The cell and the line from the TGA to the cellare operated at 200^0C.
2. When using the EGA-TGA cell please remember to turn off the heater by pressing the down arrow on the controller until the set point reads "off". You will be shown how to do this during training.
3. User are NOT cleared to change out fixtures. Only lab personnel are allowed to install or remove the ATR, the pellet holder, the EGA-TGA Cell or any other fixtures. We recommend that you notify lab personnel the day before your scheduled measurement to ensure it is ready.
4. For measuring KBr pellets: Users are expected to make/have their own pellet equipment. This includes the punch and die, the KBr, mortar and pestle, and any other equipment you deem necessary.
5. Do not attempt to "fix" or adjust or calibrate any part of the instrument or software. If you need a different configuration, please notify lab personnel of your specific needs and we will make every attempt to accommodate you.

H. APPLICATIONS:

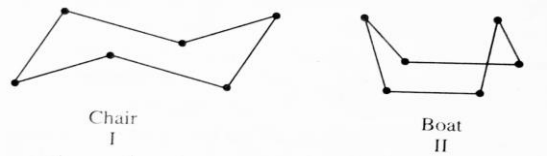
1. Identification of an organic compound.
2. Used to determine the structure of an unknown compound.
3. To perform the qualitative analysis of functional group.
4. To distinguish between the types of hydrogen bonding.
5. Helps to make the quantitative estimation of an organic mixture.
6. This technique is quite useful for studying chemical reactions.



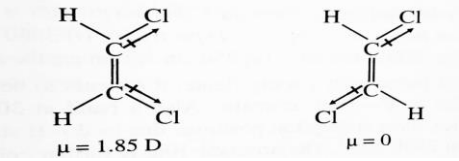
7. Study of Keto-enol tautomerism.



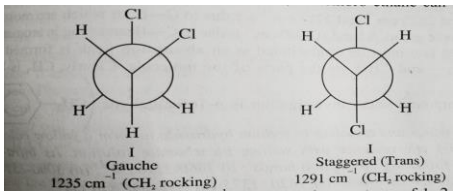
8. This technique is also useful to establish the structure of complex molecule.
9. This technique is quite useful in determining the relative stability of various conformations of cycle compounds.



10. Geometrical isomerism - This technique clearly makes a distinction between cis and trans isomers.



11. Rotational isomerism – Infra red spectroscopy helps in the determination of Gauche and staggered conformations.



12. Detection of impurities in a compound.

I. REFERENCES

1. https://www.google.com/url?sa=t&source=web&rct=j&url=https://www.thermofisher.com/in/en/home/industrial/spectroscopy-elemental-isotope-analysis/spectroscopy-elemental-isotope-analysis-learning-center/molecular-spectroscopy-information/ftir-information/ftir-applications.html&ved=2ahUKEwib9tKd_e_2AhWYT2wGHQLHAE0QFnoECBoQAQ&usg=AOvVaw1hfipZPhYTViq_uU_gUBIW
2. https://rtilab.com/techniques/ftir-analysis/#:~:text=FTIR%20analysis%20is%20used%20to,extraction%20from%20a%20polymer%20matrix
3. https://www.sciencedirect.com/topics/engineering/fourier-transform-infrared-spectrometer#:~:text=FTIR%20spectrometers%20rely %20on %20the, a%20narrow%20band%20of%20frequencies
4. Elementary Organic spectroscopy by *Y.R. Sharma, revised edition, pg.no. 76,77 & 144-147*

Dear Viewers, for further information click on the below link for Video presentation on FTIR instrumentation and interpretation::

https://youtu.be/fcVbYwX7sJ8

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