Infrared Spectroscopy

Infrared (IR) radiation is a part of the **electromagnetic spectrum**. The wavelength range extends from 0.75 µm to 1000 µm, or in **wavenumber** ($\tilde{\nu}$) from 13000 cm^{-1} to 10 cm^{-1}. This range is bordered by the red end of the **visible** region (high frequency) and the **Microwave** region (low frequency).

Region	Wavelength (λ) (µm)	Wavenumber ($\tilde{\nu}$) (cm^{-1})	Use
Near IR (NIR)	0.78−2.5	14000−4000	Used mainly for quantitative analysis to study **overtones** and **combination bands**.
Mid IR (MIR)	2.5−50	4000−400	**The most important region for chemical analysis.** Used to determine the molecular structure of organic and inorganic compounds.
Far IR (FIR)	50−1000	400−10	Used to study the vibrations of heavy atoms and lattice vibrations in solids.

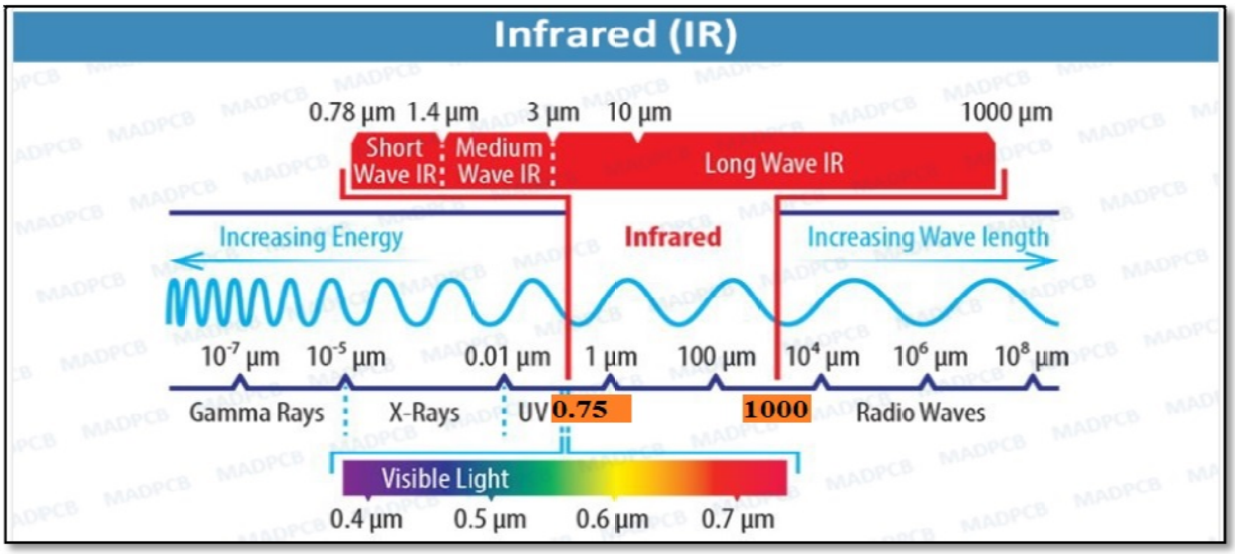
Study Regions within the MIR

The **Mid-Infrared** region is functionally divided into two critical areas:

1-Functional Group Region	**2- Fingerprint Region**
• **Range:** 4000−1450 cm^{-1} • Used to identify the presence of major functional groups (such as O-H, C=O, C≡N) because their absorption frequencies are relatively consistent. تُستخدم لتحديد وجود المجموعات الوظيفية الرئيسية (مثل O-H، C=O، و C≡N) نظرًا لثبات ترددات امتصاصها نسبيًا.	• **Range:** 1450−400 cm^{-1} • Used to **confirm the identity of a compound**, as the complex overlap of vibrations in this area produces a unique pattern (like a fingerprint) for almost every molecule. تُستخدم لتأكيد هوية المركب، حيث يُنتج التداخل المعقد للاهتزازات في هذه المنطقة نمطًا فريدًا (يشبه بصمة الإصبع) لكل جزيء تقريبًا.

The values of wavelength are converted to wavenumber and vice versa using the following relation:

$$\tilde{\nu}\ (\text{cm}^{-1}) = \frac{10000}{\lambda(\mu m)}$$



Comparison of IR and UV-Vis Spectroscopy

The absorption of molecules or materials in the IR region is not studied alongside absorption in the UV-Vis region. This is due to the following reasons:

1- Instrumentation: There are no spectrometers or devices that can cover both the UV-Vis and IR regions because the components of the spectrometers are fundamentally different.

2- Spectral Appearance (Bands):

- IR spectra yield many sharp, distinct peaks.
- UV-Vis spectra yield few, broad peaks (typically 2–4). This is because UV-Vis peaks are affected by the solvent, causing them to broaden, overlap, and thus appear few.
- In IR, the peaks do not change or broaden significantly with a change in solvent, thus maintaining their sharpness and large number.

لا يتم دراسة امتصاص الجزيئات أو المواد في منطقة **IR** مع الامتصاص في منطقة **UV-Vis** والسبب يعود إلى:

1- لا يوجد مطياف أو أجهزة يمكن أن تغطي المنطقتين (**UV-Vis** و **IR**) لأن مكونات المطياف تكون مختلفة.

2- تعطي أطياف **IR** قمم كثيرة وحادة بينما تعطي أطياف **UV-Vis** قمم عريضة وقليلة العدد بين 2-4 وذلك لأنها تتأثر بالمذيب وبالتالي تتوسع وتتداخل مع بعضها وتكون قليلة، بينما في **IR** لا تتغير أو تتوسع القمم بتغير المذيب ولهذا تحافظ على حدتها وعلى عددها الكبير.

Dipole Moment (μ)

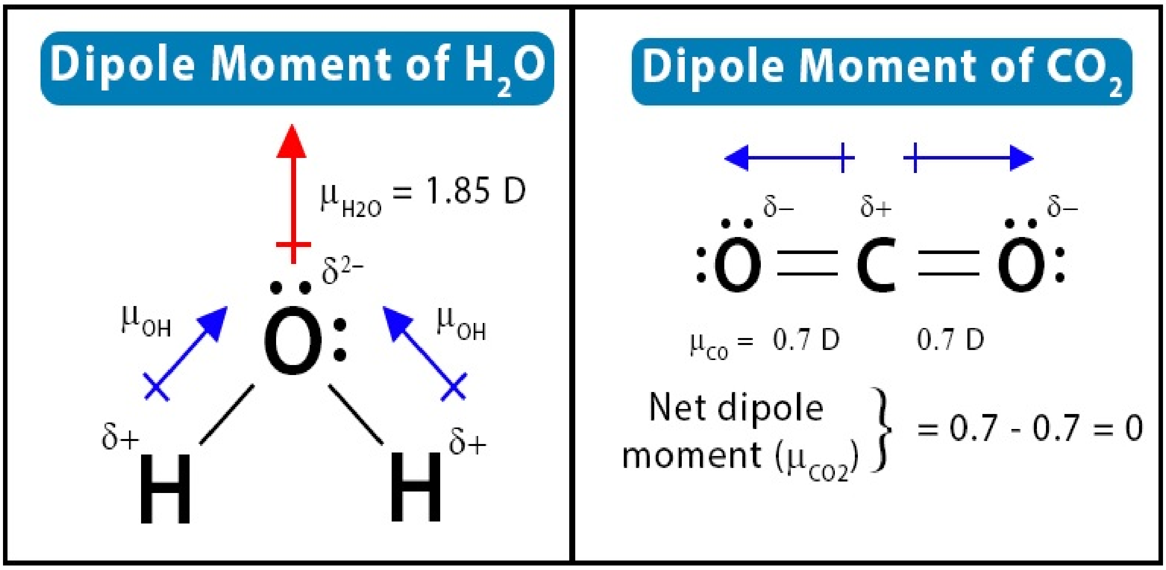
The Dipole Moment (μ) refers to the measurement of the polarity of a chemical bond or an entire molecule, and it results from the unequal distribution of electrical charge.

A dipole moment arises in a covalent bond when one atom is more electronegative than the other. This difference causes the shared electrons to spend more time around the more electronegative atom, creating a partial negative charge (δ−) on it and a partial positive charge (δ+) on the less electronegative atom.

- **Polar Molecules:** Possess a non-zero net dipole moment (such as H_2O or HCl) because the bond dipoles do not cancel each other out.
- **Non-polar Molecules:** Have a net dipole moment of zero (such as CO_2 or CH_4) because their symmetrical geometric shape causes the individual bond dipoles to cancel each other out.

Importance in IR Spectroscopy: The existence of a change in the **dipole moment** during the **vibrational motion** of the molecule is the fundamental condition for the absorption of IR radiation and the appearance of a peak in the spectrum.

إن وجود تغيير في العزم ثنائي القطب (μ) أثناء الحركة الاهتزازية للجزيء هو الشرط الأساسي لامتصاص إشعاع الأشعة تحت الحمراء (IR) وظهور قمة في الطيف.



- العزم ثنائي القطب الصافي لجزيء H_2O **لا يُلغى** ويساوي (1.85 D) لأنه جزيء ذو شكل **زاوي غير متناظر**؛ تتجه عزوم رابطتي O-H القطبية نحو الأكسجين، وحيث أنهما ليستا على خط مستقيم، فإن جمعهما الاتجاهي ينتج محصلة قطبية دائمة، مما يجعله يمتص أشعة IR بقوة.
- أما جزيء CO_2 فله عزم صافٍ **يساوي صفراً** لأنه ذو شكل **خطي** متناظر؛ فرغم أن رابطتي C=O قطبيتان، فإنهما متساويتان في المقدار ومتعاكستان تماماً في الاتجاه، فتلغي كل منهما الأخرى، مما يجعله جزيئاً لا قطبياً في حالته المستقرة، ولا يمتص IR

- Q: Why must organic compounds be dried and water removed before measurement in an IR instrument؟
- س: لماذا يتم تجفيف المركبات العضوية والتخلص من الماء قبل القياس في جهاز IR؟

أن الماء يسبب تداخلاً قوياً في طيف الأشعة تحت الحمراء (IR) ويجب تجفيف المركبات لتجنب ذلك. والسبب يُعد الماء جزيئاً قطبياً جداً وله عزم ثنائي قطب دائمي غير صفري (μ=1.85 D)، ناتج عن شكله الزاوي غير المتناظر. هذا يجعله يمتص أشعة IR بقوة في منطقتين رئيسيتين، مما يؤدي إلى تشويه الطيف:

1- منطقة اهتزازات الشد (O-H Stretching): يظهر الماء ذروة امتصاص قوية وعريضة جداً في المنطقة بين $3200–3700\ cm^{-1}$.
التداخل: تُخفي هذه القمة قمم المجموعات الوظيفية الحيوية الأخرى، مثل O-H في الكحولات والأحماض، و N-H في الأمينات، مما يشوه المعلومات الأساسية للمركب العضوي.

2- منطقة اهتزازات الانحناء (H-O-H Bending): يمتص الماء أيضاً في منطقة بصمة الإصبع الحساسة، بين $1600–1650\ cm^{-1}$ ، مما يزيد من صعوبة تفسير الطيف

Molecular Motion and Energy in IR Spectroscopy

The terms Kinetic, Vibrational, and Rotational describe three types of energy or motion a molecule possesses, which are affected by IR radiation, leading to absorption.

1. Kinetic Energy

In a broad context, the Kinetic Energy of a molecule refers to its total motion. The total energy of a molecule is composed of:

- **Translational Energy:** The movement of the molecule as a whole from one place to another.
- **Rotational Energy:** The rotation of the molecule around its axis.
- **Vibrational Energy:** The internal motion of atoms within the molecule.

IR radiation possesses sufficient energy to primarily affect the **Vibrational and Rotational** energy levels.

2. Vibrational Motion

This is the fundamental phenomenon utilized in IR spectroscopy (especially the mid-IR region). When a molecule absorbs an IR photon, it transitions from a lower vibrational state to a higher one (the amplitude of the vibration increases). Each functional group (like C=O or O-H) has a characteristic vibrational frequency, which allows IR to identify these groups.

3. Rotational Motion

This is the rotation of the entire molecule around its axis, or the rotation of molecular groups around single bonds (e.g., the rotation of a methyl group).

Essential Condition for IR Absorption

For absorption to appear in the IR spectrum, the vibrational or rotational motion (or both) must lead to a change in the Dipole Moment (μ) of the molecule during that motion. If the dipole moment does not change during the bond movement (as in symmetrical molecules like N2 or O2), no absorption will occur in the IR region.

الشرط الأساسي لامتصاص الأشعة تحت الحمراء لكي يظهر الامتصاص في طيف الأشعة تحت الحمراء، يجب أن تؤدي الحركة الاهتزازية أو الدورانية (أو كليهما) إلى تغير في عزم ثنائي القطب (μ) للجزيء أثناء تلك الحركة .إذا لم يتغير عزم ثنائي القطب أثناء حركة الرابطة (كما في الجزيئات المتماثلة مثل N2 أو O2) ، فلن يحدث أي امتصاص في منطقة الأشعة تحت الحمراء.

Types of Molecular Vibrations in IR Spectroscopy

Molecular vibrations in Infrared (IR) Spectroscopy are primarily divided into two categories: **Stretching** and **Bending**.

1. Stretching Vibrations الاهتزازات الامتطاطية

These vibrations involve changes in the **bond length** along the axis of the bond. They require **higher energy** and occur at **higher wavenumbers** $\tilde{\nu}$ in the IR spectrum (typically in the 4000–1300 cm^{-1} region).

Type	**Description**
Symmetric Stretching متماثل	Both atoms bonded to the central atom move **in and out simultaneously** and in the same direction.
Asymmetric Stretching غير متماثل	One bonded atom moves **in** while the other moves **out** (i.e., in opposite directions).

2. Bending Vibrations الاهتزازات الانحنائية

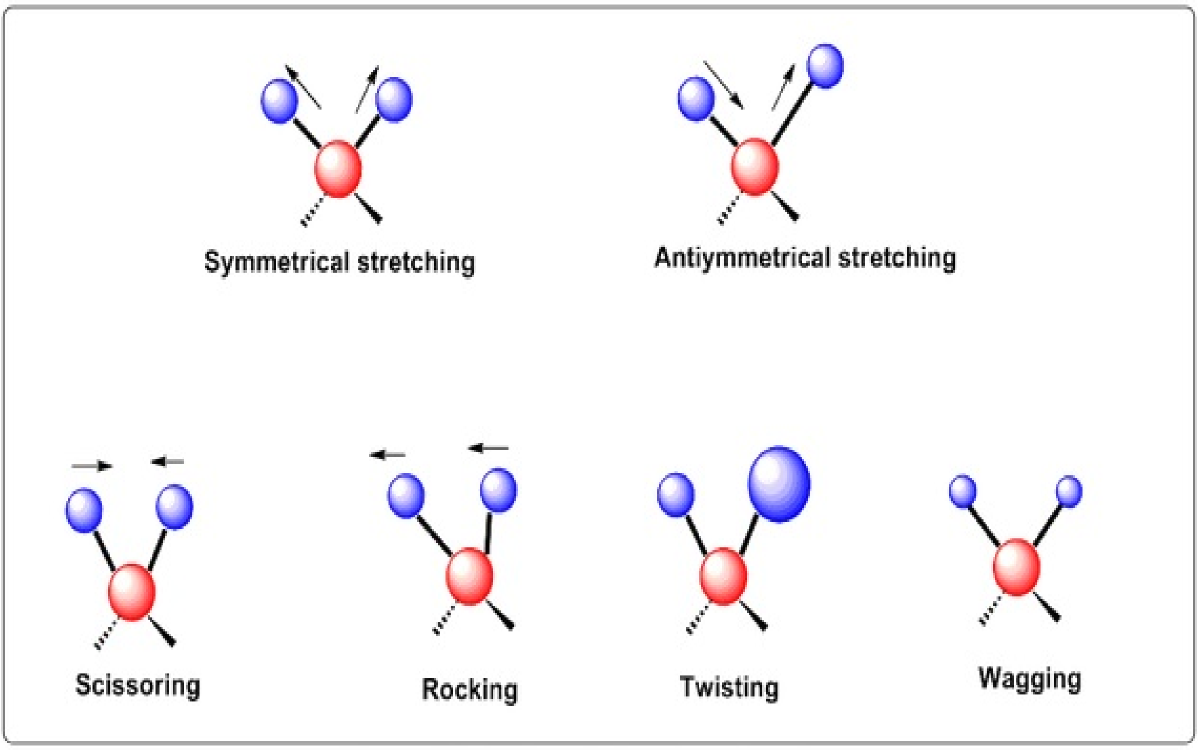
These vibrations involve changes in the **angle between bonds**, rather than the bond length. They require **lower energy** and occur at **lower wavenumbers** (ν~) (usually in the sensitive **Fingerprint Region**, 1300–650 cm^{-1}).

Bending vibrations are further categorized into four sub-types

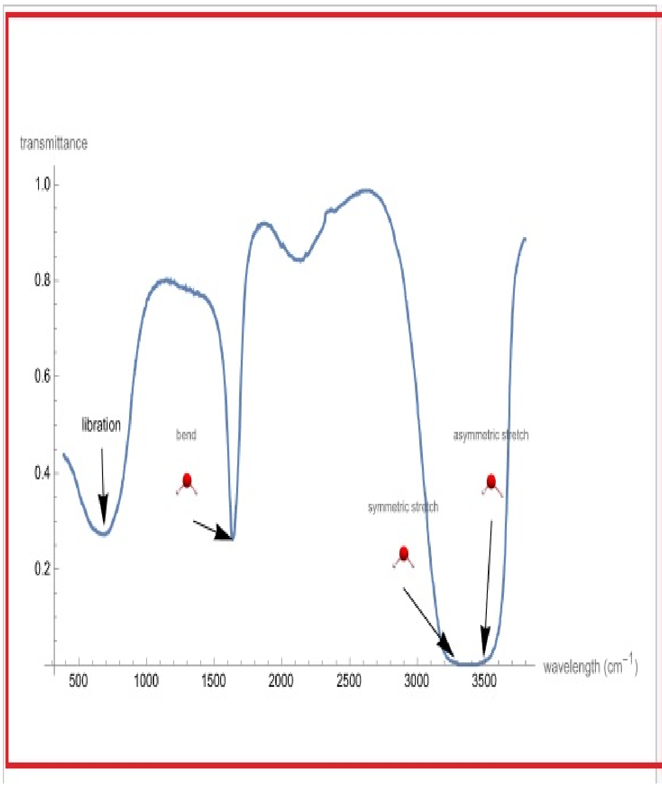
Type	Direction	Description
Scissoring مقصي	**In-plane** داخل المستوى	The two bonded atoms move **towards and away** from each other (like scissor blades).
Rocking تأرجحي	**In-plane** داخل المستوى	The two bonded atoms move **together** from side-to-side (swinging).
Wagging ارتجاجي	**Out-of-plane** **خارج المستوى**	The two bonded atoms move **together** up and down relative to the molecular plane.
Twisting التوائي	**Out-of-plane** **خارج المستوى**	One bonded atom moves **up** while the other moves **down** relative to the molecular plane.

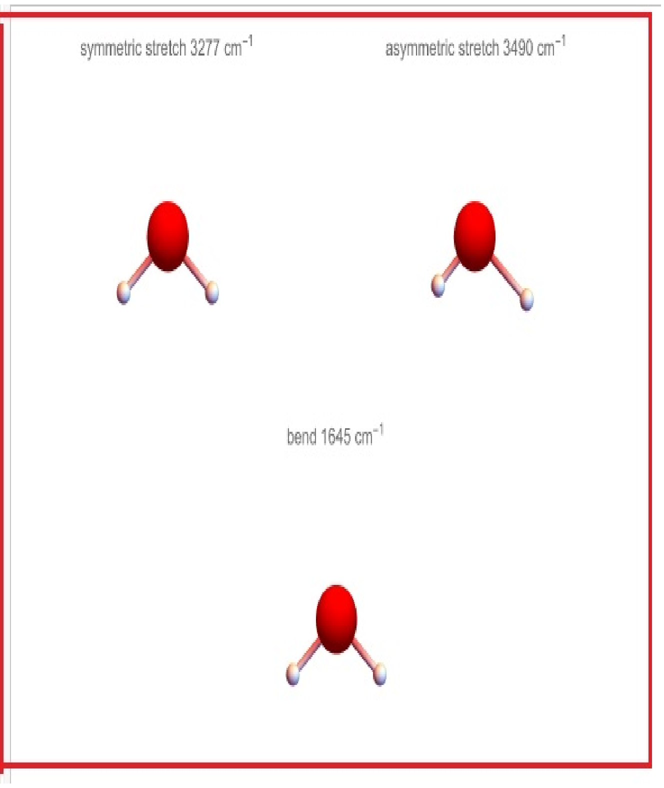
Note on Significance

Stretching is generally the most important type of vibration in the **functional group region** (4000–1300 cm^{-1}) because it is used to identify key chemical groups (C=O, O-H, etc.).



Types of vibrations in Organic molecules





Hooke's Law in IR Spectroscopy

Hooke's Law provides the fundamental physical model for understanding molecular vibrations in Infrared (IR) spectroscopy.

$$\tilde{\nu}=\frac{1}{2\pi c}\sqrt{\frac{k}{\mu}}$$

Where:

- $\tilde{\nu}$: **Wavenumber** (cm^{-1}), representing the position of the absorption peak.
- k: **Force Constant** (dyne/cm), representing the strength/stiffness of the chemical bond.
- μ: **Reduced Mass** (g), representing the effective mass of the two atoms.
- c: Speed of light (3×10^{10} cm/sec).

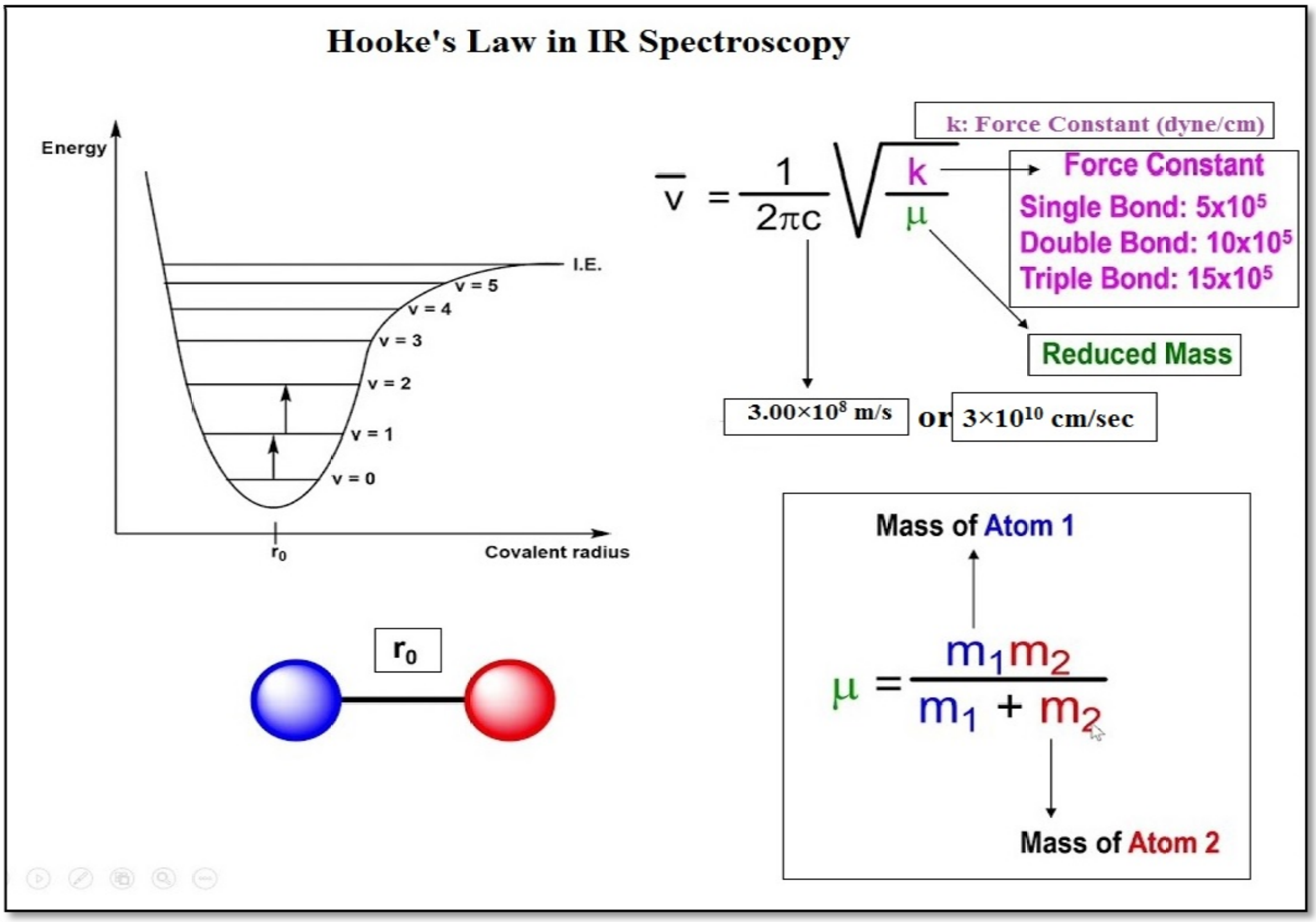
The reduced mass (μ) is calculated from the atomic weights of the two atoms (M1 and M2):

$$\mu=\frac{M1\times M2}{M1+M2}$$

The Hooke's Law equation shows that the vibrational energy (and thus the wavenumber $\tilde{\nu}$ is primarily governed by two factors: **bond strength** and **atomic mass**.

<table>
<tr><th>Factor</th><th>Relationship to $\tilde{\nu}$</th><th>Effect on Absorption</th></tr>
<tr><td>Bond Strength (k)</td><td>Directly Proportional
$\tilde{\nu}\propto\sqrt{k}$</td><td>Stronger bonds (higher k) result in higher wavenumbers. For example, Triple Bonds (C≡C) absorb at higher $\tilde{\nu}$ than Double Bonds (C=C), which absorb higher than Single Bonds (C−C).</td></tr>
<tr><td colspan="3">القاعدة الأولى: تأثير قوة الرابطة(k) :الروابط الأقوى (ذات ثابت القوة kالأعلى) تؤدي إلى أعداد موجية ($\tilde{\nu}$) أعلى. على سبيل المثال، تمتص الروابط الثلاثية (C≡C) عند عدد موجي أعلى من الروابط المزدوجة (C=C) ، والتي بدورها تمتص عند عدد موجي أعلى من الروابط الأحادية.(C−C) حيث ان:
• قيم kالتقريبية الموضحة:
• (C−C) (Single Bond): 5×10^{5}
• (C=C) (Double Bond): 10×10^{5}
• (C≡C) (Triple Bond): 15×10^{5}</td></tr>
</table>

Reduced Mass (μ)	**Inversely Proportional** $\tilde{\nu} \propto \frac{1}{\sqrt{\mu}}$	**Lighter atoms** (lower μ) result in **higher wavenumbers**. For example, C-H bonds absorb at much higher $\tilde{\nu}$ than C-Cl bonds because the hydrogen atom is much lighter.
القاعدة الثانية: تأثير الكتلة المختزلة (μ): الذرات الأخف (ذات الكتلة المختزلة μالأقل) تؤدي إلى أعداد موجية ($\tilde{\nu}$) أعلى. على سبيل المثال، تمتص روابط C-H عند عدد موجي أعلى بكثير من روابط C-Cl لأن ذرة الهيدروجين أخف بكثير.		


Hooke's Law in IR Spectroscopy

$$\bar{\nu} = \frac{1}{2\pi c}\sqrt{\frac{k}{\mu}}$$

k: Force Constant (dyne/cm)

Force Constant
Single Bond: 5×10^5
Double Bond: 10×10^5
Triple Bond: 15×10^5

Reduced Mass

3.00×10^8 m/s or 3×10^{10} cm/sec

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

Mass of Atom 1

Mass of Atom 2

Question: Calculate the **reduced mass (μ)** for the C-H bond. (Assume the atomic mass of Carbon (C) is 12 g/mol and Hydrogen (H) is 1 g/mol).

Answer:

$$\mu = \frac{M1 \times M2}{M1 + M2}$$

$$\mu = \frac{12 \times 1}{12 + 1} = \qquad \mu \approx 0.923 \text{ g/mol}$$

Question: The image shows that the Force Constant (k) for a double bond is approximately 10×10^5 dyne/cm, and for a single bond, it is 5×10^5 dyne/cm. **Calculate the vibrational frequency ($\bar{v}$) of a C=O double and C-O single bond?** The reduced mass (μ) for the C-O bond is calculated using the atomic masses of Carbon ($M_C \approx 12.0$ g/mol) and Oxygen ($M_O \approx 16.0$ g/mol)

Answer:

$$\mu = \frac{M1 \times M2}{M1 + M2}$$

$$\mu = \frac{12 \times 16}{12 + 16} = \frac{\mathbf{192}}{\mathbf{28}} \qquad \mu \approx 6.86 \text{ g/mol}$$

Reduced Mass in grams (μ): To use the full formula, we use the fact that ($\mu = \frac{\mu_{mol}}{N_A}$), where NA is Avogadro's number (6.022×10^{23} mol^{-1}).

يتم يتحويل وحدات الكتلة المختزلة الى غرام من خلال تقسيم الكتلة المختزلة على عدد افوكادروا

$$\mu = \frac{6.86 \text{ g/mol}}{6.022 \times 10^{23} \text{mol}^{-1}} = 1.139 \times 10^{-23} \text{ g}$$

$$\tilde{v} = \frac{1}{2\pi c}\sqrt{\frac{k}{\mu}}$$

1- For C-O single bond, k= 5×10^5 dyne/cm=5×10^5 g/s^2

$$\tilde{\upsilon}=\frac{1}{2(3.14)(3\times10^{10}\ \mathrm{cm/sec})}\sqrt{\frac{5\times10^{5}\ \mathrm{g/s2}}{1.139\times10^{-23}\ \mathrm{g}}}$$

$$\widetilde{\upsilon_{c-o}}\approx 1{,}112\ \mathrm{cm}^{-1}$$

2- For C=O single bond, k= 5×10^{10} dyne/cm=5×10^{10} g/s^2

$$\tilde{\upsilon}=\frac{1}{2(3.14)(3\times10^{10}\ \mathrm{cm/sec})}\sqrt{\frac{5\times10^{10}\ \mathrm{g/s2}}{1.139\times10^{-23}\ \mathrm{g}}}$$

$$\widetilde{\upsilon_{c=o}}\approx 1{,}572\quad \mathrm{cm}^{-1}$$

Q/ Calculate the reduced mass (μmol) in g/mol for a Carbon-Hydrogen (C−H) bond, using the approximate atomic masses: $M_C\approx12.0$ g/mol and $M_H\approx1.0$ g/mol.

Q/ the reduced mass (μ_{mol}) for a C−H bond is approximately 0.923 g/mol. If the force constant (k) for a single bond is k≈5×10^{5} dyne/cm, what is the estimated vibrational frequency ($\bar{\nu}$) of the C−H stretch in cm^{-1}? (Use c=3.00×10^{10} cm/s and NA =6.022×10^{23} mol^{-1})

Factors Affecting Bond Vibration

1- Bond Elasticity (Force Constant K)

Bonds connecting heavy atoms have a large reduced mass (μ) and vibrate at a low frequency. Conversely, bonds connecting light atoms vibrate at a higher frequency because μ will be small. Triple bonds are stronger than double and single bonds for the same atoms, and therefore have a high vibrational frequency. Thus, as the Force Constant (K) increases, the bond strength increases.

Bond	**Frequency $\tilde{\nu}$**	
C≡C	2150 cm^{-1}	↑ **Increasing K**
C=C	1650 cm^{-1}	
C−C	1200 cm^{-1}	
	قيم k التقريبية الموضحة: (C−C) **(Single Bond):** 5×10^5 (C=C) **(Double Bond):** 10×10^5 (C≡C) **(Triple Bond):** 15×10^5	

2-Reduced Mass (μ) of Bonded Atoms:

The following relationship demonstrates that the reduced mass (μ) increases **as the mass of the atoms bonded to the carbon atom increases, consequently causing a** decrease in the vibrational frequency **$(\bar{\nu})$.**

Bond	**Frequency $\tilde{\nu}$**	
C−H	3000 cm^{-1}	↓ **μ Increasing**
C−C	1200 cm^{-1}	
C−O	1100 cm^{-1}	
C−Cl	800 cm^{-1}	
C−Br	550 cm^{-1}	
C−I	500 cm^{-1}	
ارتفاع العدد الذري لليود يعني ارتفاع كتلته، وهذا هو السبب الرئيسي وراء **انخفاض تردد اهتزاز آصرة C−I**		

3- Hybridization:

Hybridization affects the Force Constant (K), **and the bond strength follows the sequence:**

Sp>Sp2>Sp3

The following frequencies (for the C−H bond) illustrate this:

Bond	**Hybridization**	**Frequency $\tilde{\nu}$**
≡C−H	**Sp**	3300 cm^{-1}
=C−H	**Sp2**	3100 cm^{-1}
−C−H	**Sp3**	2900 cm^{-1}

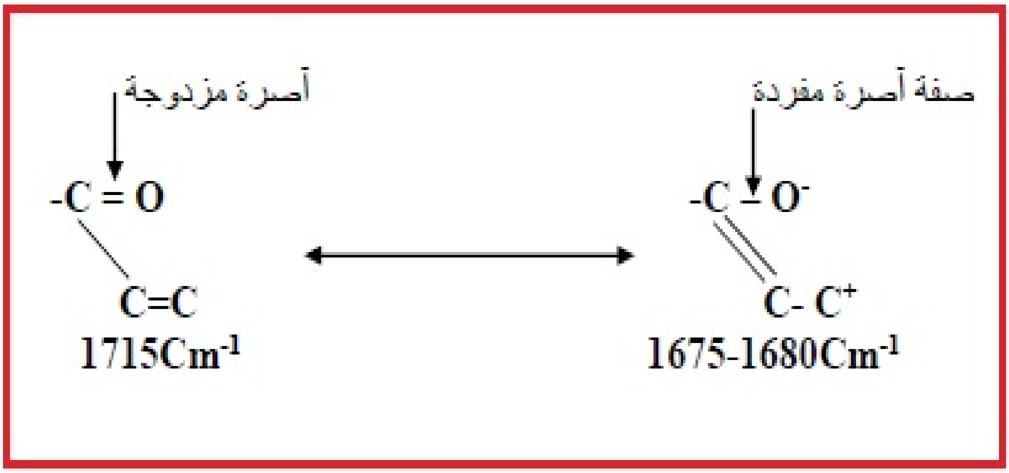
4-Resonance

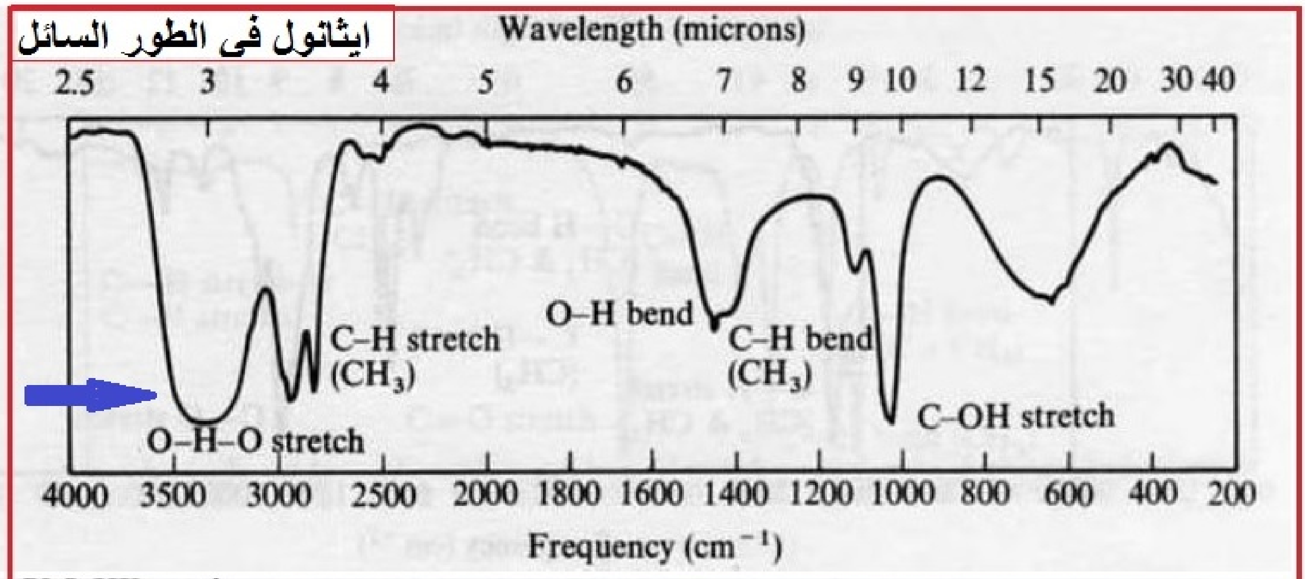
Resonance affects the strength and length of the bond, and consequently the value of the **force constant (K)**.

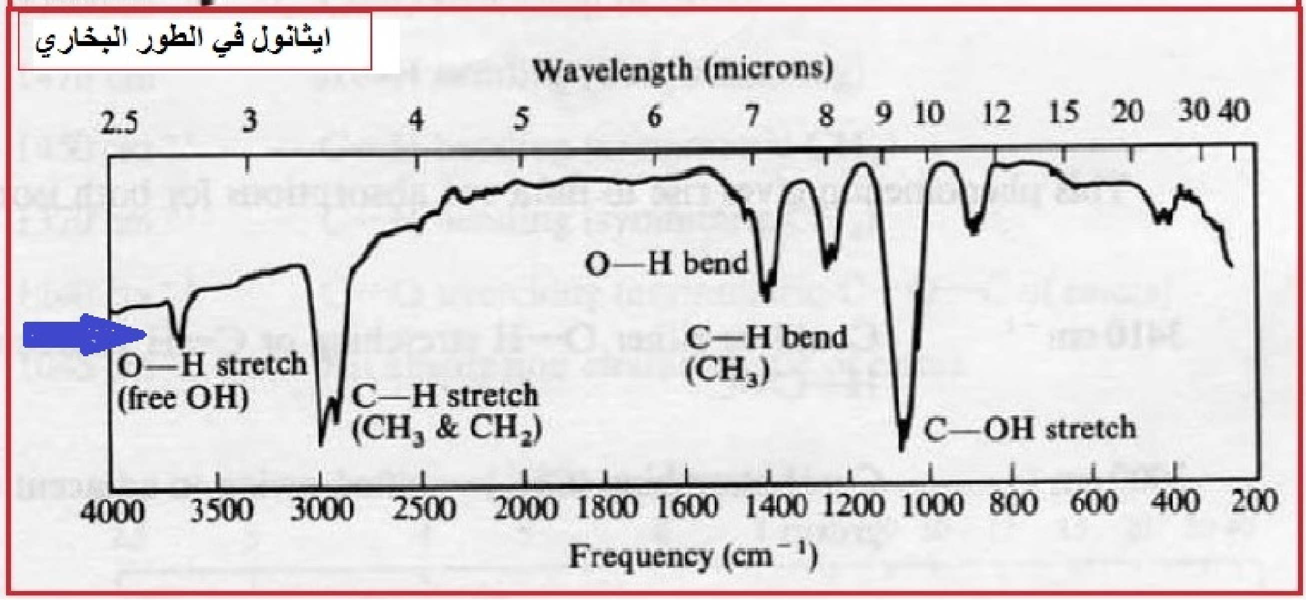
The carbonyl group (C=O) in a simple ketone has a stretching vibrational frequency of ≈**1715 cm^{-1}**.

However, when this group is linked to a double bond (i.e., in a state of **conjugation** with the carbonyl), it vibrates at a lower frequency, ≈**1675−1680 cm^{-1}**.

This drop in frequency is due to **resonance**, which causes the C=O bond to **elongate** (become longer) and gives it more **single-bond character** than double-bond character. This results in a **decrease in bond strength** and a decrease in the force constant (K). Consequently, the vibrational frequency ($\bar{v}$) is lowered.





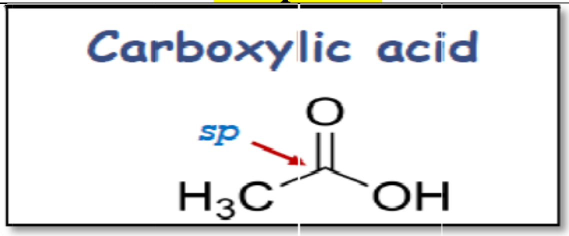
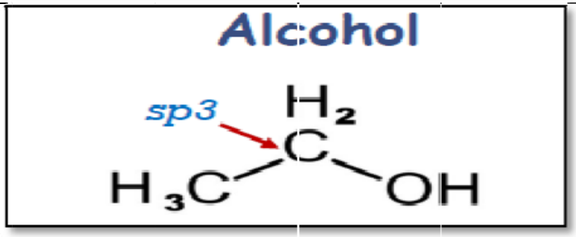
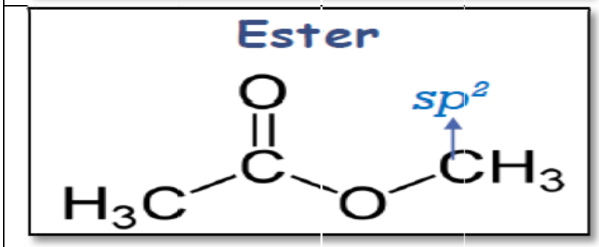
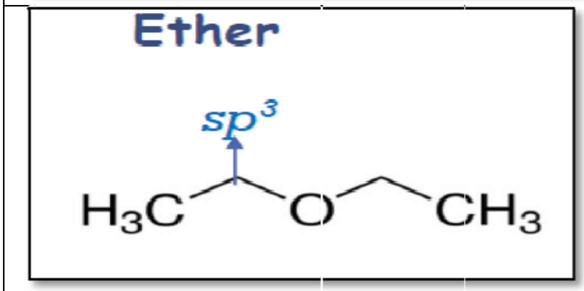
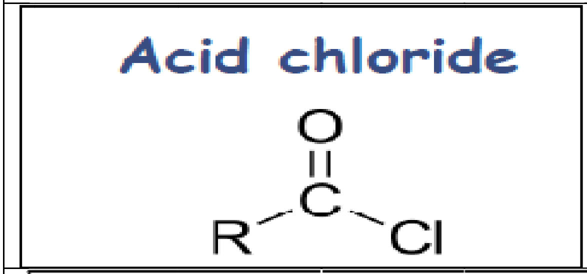
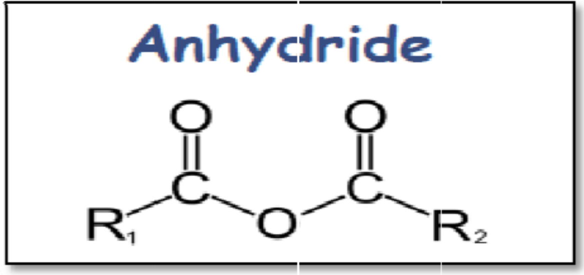


طيف الميثانولCH_3OH في الطور السائل liquid phase نلاحظ قمة O-H عريضة وأكثر شدة وأقل عدد موجي مما في الايثانول الذي أخذ له طيف IR في الطور البخاري vapour phase بسبب الآصرة الهيدروجينية التي تعمل على أضعاف الآصرة وبالتالي نقصان قيمة k

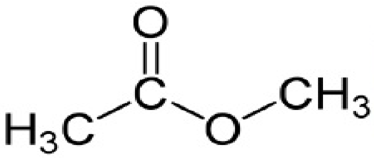
في طيف IR للايثانولCH_3OH في الطور البخاري phase vapor نلاحظ تردد مط مجموعة OH حادة وأقل شدة وأكبر عدد موجي بسبب حرية OH في الطور البخاري

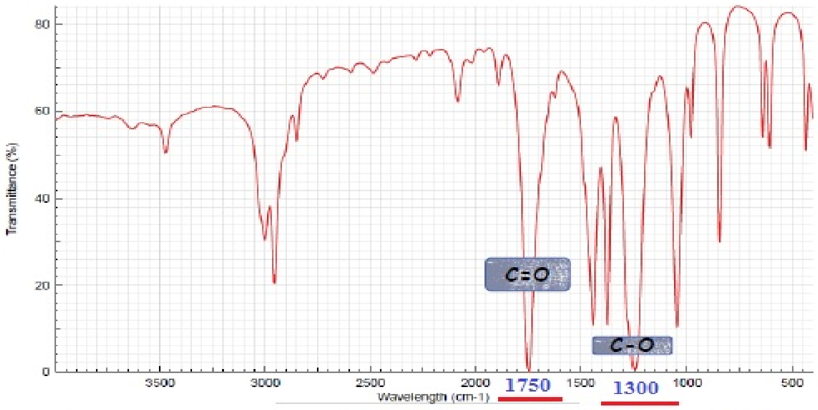
Example of Vibrations in IR Spectroscopy

The frequency range for the stretching vibration depends on the type of molecule and whether hydrogen bonding is present

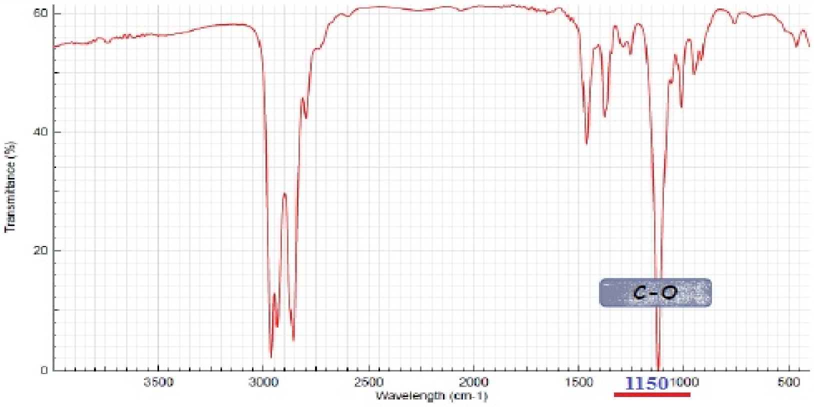
compound	C=O	O-H	C−O
	**1700 cm^{-1}**	**2500−3300 cm^{-1}**	**1210-1320 cm^{-1}**
	**-**	**3200-3500 cm^{-1}**	**1000-1150 cm^{-1}**
	**1735-1750 cm^{-1}**	**-**	**1000-1300 cm^{-1} two bond**
	**-**	**-**	**1000-1150 cm^{-1}**
	**1790-1810 cm^{-1}**	**-**	**-**
	**1750-1800 cm^{-1}**	**-**	**900-1300 cm^{-1}**

Ester

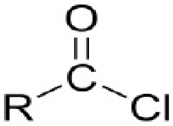


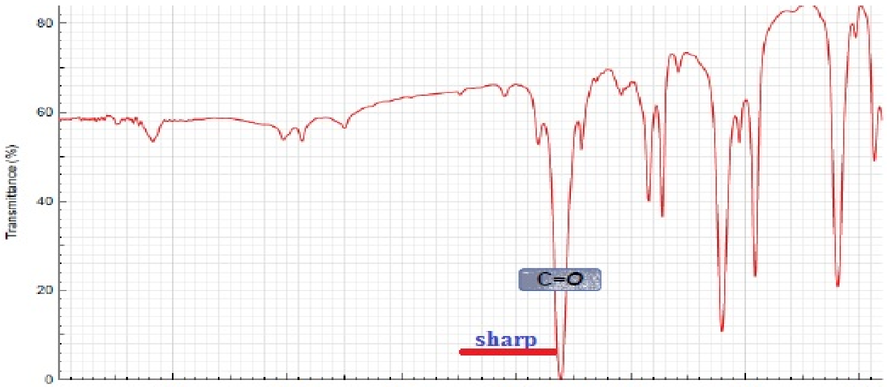


Ether

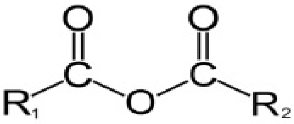


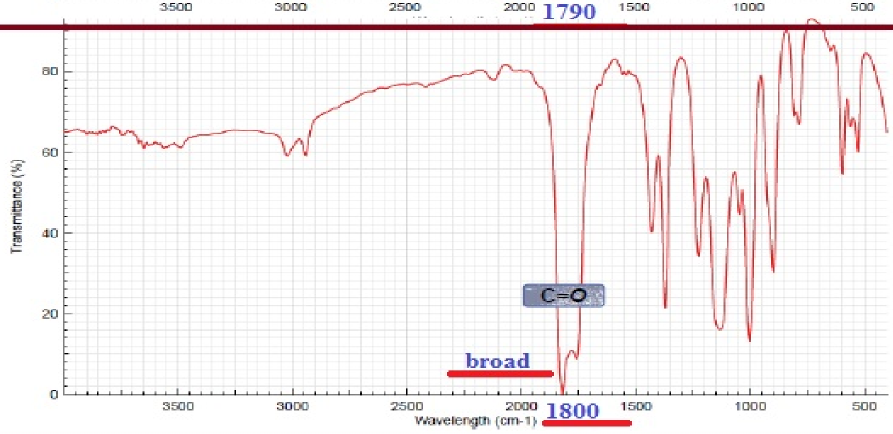
Acid Chloride

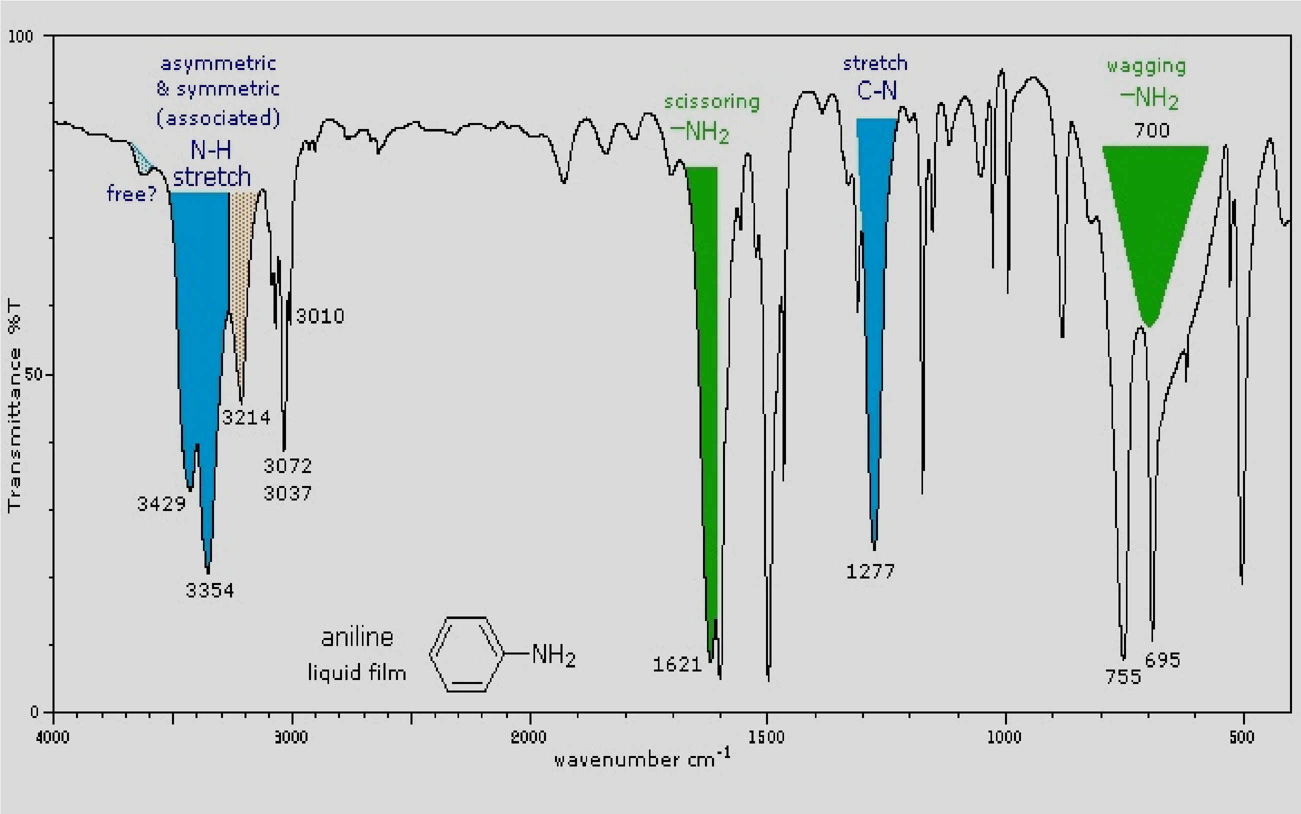


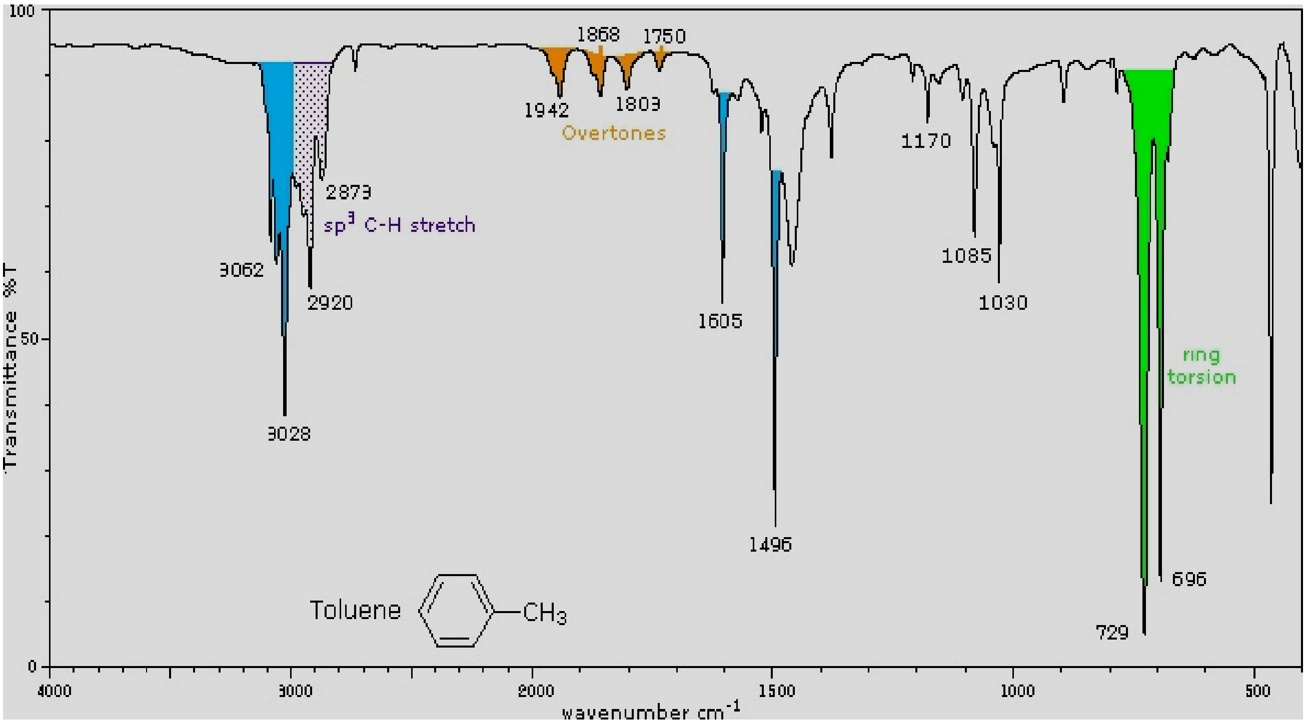


Anhydride






100
50
0
Transmittance %T
asymmetric
& symmetric
(associated)
N-H
stretch
free?
3429
3354
3214
3072
3037
3010
scissoring
−NH2
1621
stretch
C-N
1277
wagging
−NH2
700
755
695
aniline
liquid film
NH2
4000
3000
2000
1500
1000
500
wavenumber cm-1

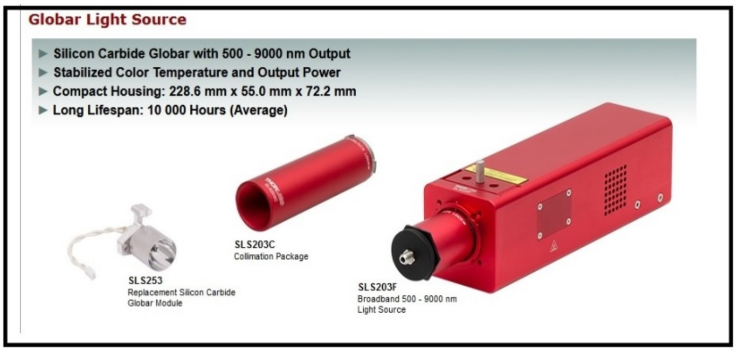

100
50
0
Transmittance %T
1868
1750
1942
1803
Overtones
2873
sp3 C-H stretch
3062
2920
3028
1605
1496
1170
1085
1030
ring
torsion
696
729
Toluene
CH3
4000
3000
2000
1500
1000
500
wavenumber cm-1

IR Spectrophotometer

The functional components of an IR spectrometer are:

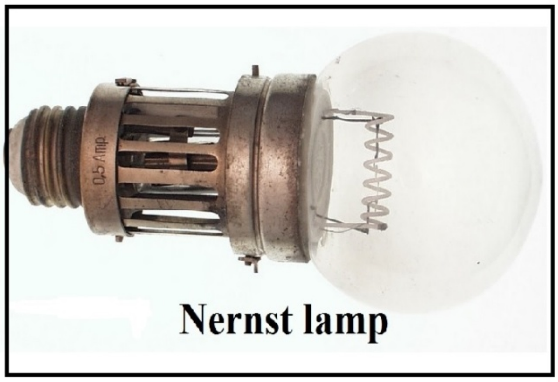
1. **IR Radiation Source:** Generates the infrared radiation necessary to excite molecular bond vibrations. like

sources of IR radiations		
Nernst glower مصباح نيرنست	Incandescent lamp مصباح متوهج	Mercury arc قوس زئبقي
Tungsten lamp مصباح تنغستن	Glober source (Silicon Carbide rod). مصباح غلوبار قضيب كربيد السيليكون	Nichrome wire سلك نيكروم

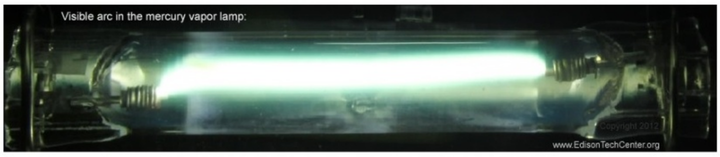


Globar Light Source

- Silicon Carbide Globar with 500 - 9000 nm Output
- Stabilized Color Temperature and Output Power
- Compact Housing: 228.6 mm x 55.0 mm x 72.2 mm
- Long Lifespan: 10 000 Hours (Average)



Nernst lamp



Mercury Vapor Lamps

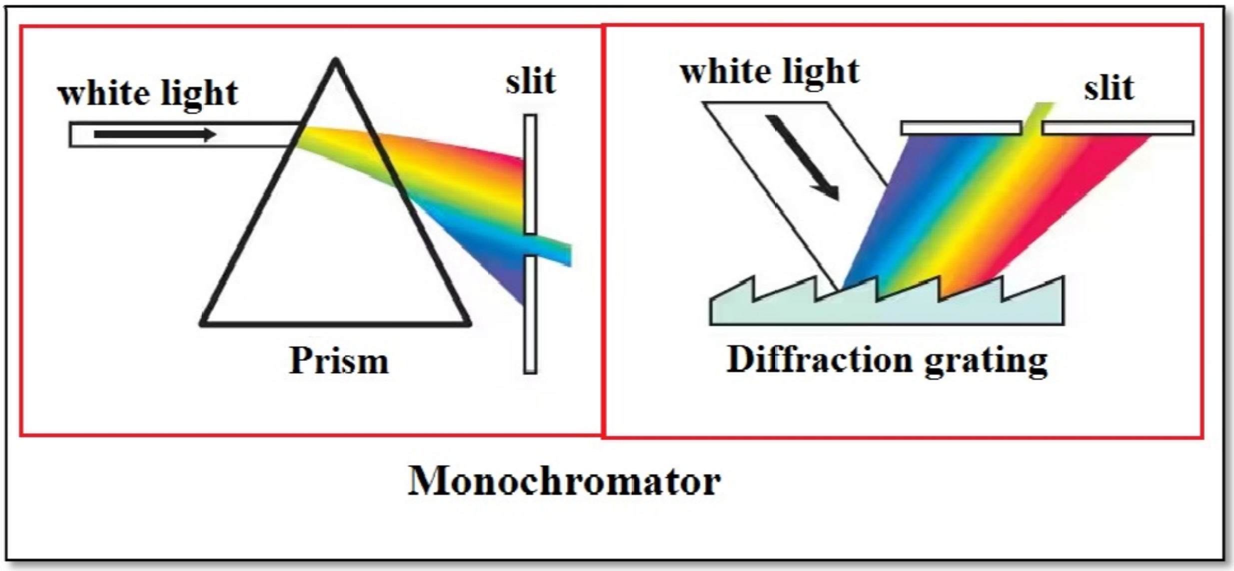
2. **Sample Cell/Compartment:** Where the sample is placed. Cells are typically made of salt crystals (like KBr or NaCl) because glass absorbs IR radiation.

Sample Cell/Compartment		
Solid sample	**Liquid samples**	**Gas samples**
• **Pressed pellets:** A solid is ground with KBr and pressed into a thin disk. • **Mull technique:** The solid is ground into a paste with a non-volatile liquid like Nujol. • **Thin films:** A thin film can be cast from a solution. • **Diffuse reflectance:** A technique that requires very little sample preparation.	• A thin film of the liquid is sandwiched between two infrared-transparent salt plates (like NaCl). • Solvents are often used, but care must be taken to avoid absorption bands that overlap with the sample's spectrum. • **ATR:** Allows direct measurement of liquids on the crystal surface.	• The gas is contained in a special cell. • Sampling is similar to liquids, but the sample is in the gaseous state within the cell. • IR spectroscopy can be used to monitor gas composition in applications like emissions monitoring.

Preparation solid sample using KBr Pellet Press

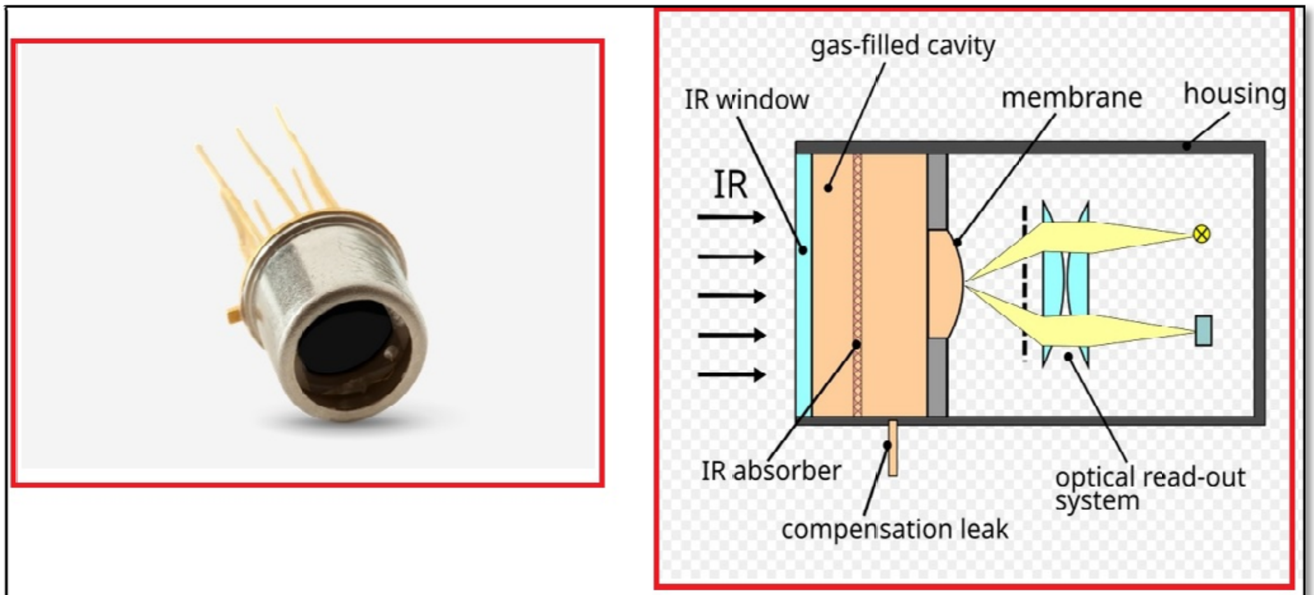
3. **Wavelength Analyzer (Monochromator):** Various types of monochromators are prism, diffraction gratings and filters.

Monochromator made of:		
Prisms المنشورات	**Diffraction gratings** محززات الحيود	**Filters** المرشحات
Potassium bromide, Sodium chloride or Caesium iodide , which refract different wavelengths at different angles.	alkali halides , which used for dispersing light, but by using diffraction.	Lithium Fluoride , which used to block certain wavelengths and allow others to pass through.



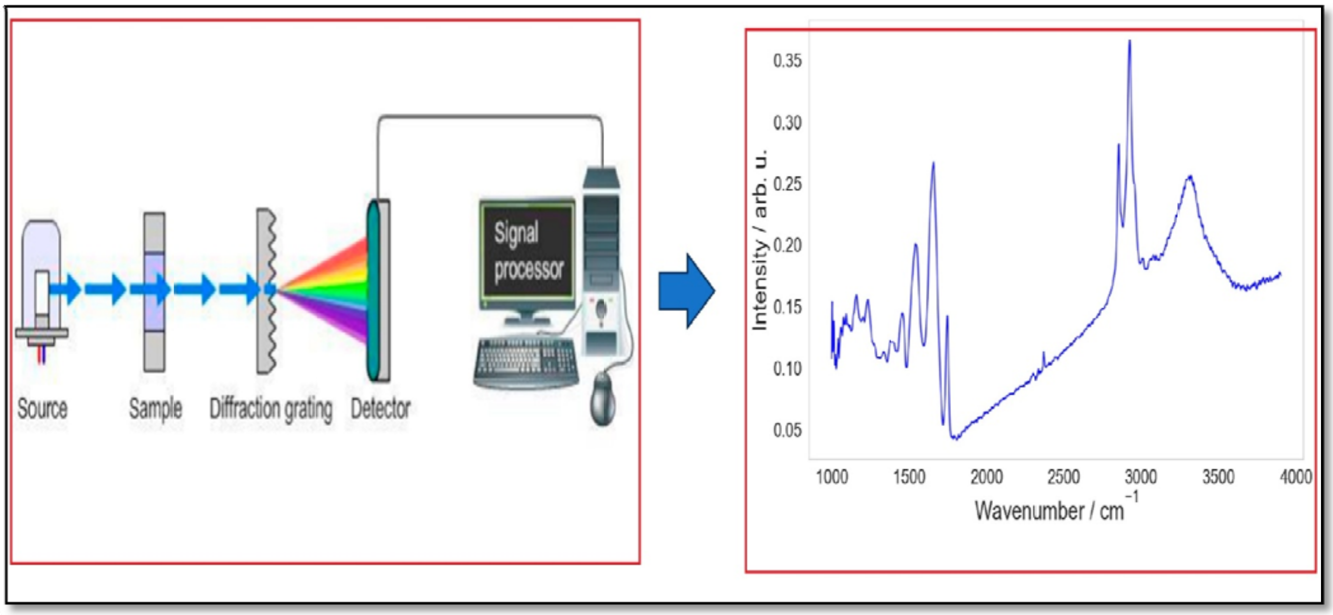
4. **Detectors:** Detectors are used to measure the intensity of unabsorbed infrared radiation. Detectors like thermocouples, Bolometers, thermistors, Golay cell, and pyro-electric detectors are used.

Detectors				
Thermocouple المزدوج الحراري	**Bolometer** مقياس البولوميتر	**Thermistor** الثرمستور	**Golay cell** خلية جولاي	**Pyro-electric detector** كاشف كهربائي حراري
thermocouple consists of two different metals joined at a junction. When this junction is heated by IR radiation, the temperature difference between the junction and a reference junction creates a voltage, which is then measured as an .electrical signal	A bolometer measures the change in its electrical resistance caused by the temperature increase from absorbing IR radiation. The blackened absorber converts the radiation into heat, which changes the resistance of the sensing .element	Similar to a bolometer, a thermistor is a type of semiconductor resistor whose resistance is highly dependent on temperature. When IR radiation heats the thermistor, its resistance changes, providing a signal	A Golay cell has a small cavity filled with a gas that absorbs IR radiation. When radiation enters the cell, it heats the gas, causing it to expand and push against a flexible membrane with a mirror attached. The movement of this membrane is measured to indicate the intensity of the radiation.	These detectors are made of a thin crystal, such as deuterated tryglycine sulfate (DTGS) or lithium tantalate. They are sensitive to changes in temperature. The IR radiation causes a change in the detector's temperature, which in turn alters the pyroelectric properties of the crystal, generating an electrical signal.



Golay cell

5. **Signal Processor/Recorder:** Processes the electrical signal and converts it into the IR spectrum (a plot of **intensitiy vs. wavenumber (cm^{-1})**).



The difference between IR, FTIR, and ATR

The difference between IR (Infrared Spectroscopy), FTIR (Fourier-Transform Infrared Spectroscopy), and ATR (Attenuated Total Reflectance) lies in their technology and sampling technique.

1. IR (Infrared Spectroscopy)

Technology: Originally referred to Dispersive IR instruments, which use a monochromator (like a prism or grating) to separate the IR beam into individual frequencies before they reach the detector.

It measures the interaction of IR radiation with matter to study molecular vibrations.

2. FTIR (Fourier-Transform Infrared)

Technology: Uses an Interferometer (specifically a Michelson interferometer) instead of a monochromator. The interferometer splits the beam, and the detector receives an interferogram (a complex signal containing all frequencies simultaneously).

Data Processing: The interferogram is converted into the final spectrum (Absorption vs. Wavenumber) using a mathematical process called the Fourier Transform.

Speed (Jacquinot's Advantage): It collects the entire spectrum in a fraction of a second, making it much faster.

Sensitivity (Fellgett's Advantage): It has a much higher signal-to-noise ratio.

Accuracy (Connes' Advantage): It provides superior wavelength precision.

Q/ What are the three primary advantages that make FTIR superior to traditional dispersive IR spectroscopy?

Answer/

Speed (Jacquinot's Advantage)	**ميزة السرعة (ميزة جاكينو)**	يقوم الجهاز بجمع الطيف كاملاً في جزء من الثانية، مما يجعله أسرع بكثير من الأجهزة التشتيتية.
Sensitivity (Fellgett's Advantage)	**ميزة الحساسية (ميزة فيلجيت)**	يمتلك الجهاز نسبة إشارة إلى ضوضاء (S/N) أعلى بكثير، مما يعني أن حساسيته أكبر.
Accuracy (Connes' Advantage)	**ميزة الدقة (ميزة كونيس)**	يوفر الجهاز دقة فائقة في تحديد الأطوال الموجية/الترددات (Wavelength/Wavenumber Precision

3. ATR (Attenuated Total Reflectance)

Principle: It relies on the phenomenon of Total Internal Reflection. The IR beam is directed onto a highly reflective crystal (e.g., Diamond, ZnSe). When the sample is pressed onto the crystal, the IR light penetrates only a very short distance (usually 0.5 to 2 micrometers) into the sample, creating an evanescent wave.

Key Feature: It allows analysis of samples directly (solids, liquids, powders) with minimal to no sample preparation.

Advantage: Eliminates the need for traditional preparation methods like KBr pellets or thin films.

Term	Category التصنيف	Function / Technology المبدأ البصري	Typical Sample Requirement تحضير العينة	work
IR (Infrared Spectroscopy) (التشتيتي)	General Technique / Dispersive Instrument التقنية الأساسية/الجهاز القديم	Measures absorbance by sequentially scanning frequencies. يستخدم موحد اللون **(Monochromator)** كالمحززات لفصل الترددات **sequentially** تتابعياً.	Requires sample preparation (KBr pellet, liquid cell). يتطلب تحضيراً تقليدياً مثل أقراص **KBr**، أو طبقات رقيقة، أو خلايا سائلة.	• يقيس شدة الإشعاع لكل تردد منفصل. • أبطأ وأقل حساسية نسبة الإشارة إلى الضوضاء أقل
FTIR (Fourier-Transform Infrared) (تحويل فورييه)	Instrument Type (Advanced IR) المتقدم	Measures all frequencies simultaneously using an **Interferometer** and **Fourier Transform** math. يستخدم مقياس التداخل **(Interferometer)** لقياس جميع الترددات في وقت واحد.	Requires sample preparation يتطلب تحضيراً تقليدياً	• يستخدم تحويل فورييه **(Fourier Transform)** لتحويل إشارة التداخل **(Interferogram)** إلى طيف. • أسرع بكثير ميزة جاكينوت • وأكثر حساسية ميزة فيلجيت • دقة عالية، سرعة فائقة، وقدرة على قياس التفاعلات السريعة
ATR (Attenuated Total Reflectance) (الانعكاس الكلي المخفف)	Sampling Accessory تقنية/ملحق أخذ العينات	Measures the absorption of an **evanescent wave** created by total internal reflection at a crystal surface. يعتمد على الانعكاس الكلي الداخلي داخل بلورة (عادة الماس)، حيث يخترق الإشعاع العينة بعمق قليل جداً (موجة زائلة).	sample is pressed directly onto the crystal. لا يتطلب تحضيراً؛ توضع العينة الصلبة أو السائلة مباشرة على سطح البلورة.	• يقيس الامتصاص عبر الموجة الزائلة. • سريع جداً حيث يلغي الحاجة لتحضير العينة. • مثالي للتحليل السريع للمواد السميكة والمعتمة واللزجة **(Paste)**، **Thick opaque polymer film** • والتحليل في الموقع.

Q/Compare and contrast Dispersive IR and FTIR spectroscopy ?

Q/Define ATR (Attenuated Total Reflectance) and explain how it differs from traditional transmission IR sampling.

Q/ For which of the three techniques is sample preparation (e.g., making a KBr pellet) typically unnecessary? Explain the principle that makes this possible.

Q/You have a thick, opaque polymer film to analyze. Which technique (ATR or traditional FTIR with transmission cell) would you choose, and why?