UCB008 - APPLIED CHEMISTRY

Infra-red Spectroscopy Series
Lecture - I

IR Spectroscopy - Introduction

by

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Learning Outcomes

At the end of this session participants should be able to:

- Identify an IR spectrum of a compound

- Understand relationship between vibrational transitions and IR spectroscopy

Microwave Spectroscopy

- Rotational energy level transitions of the gaseous molecules on the absorption of radiations falling in microwave region.

- Molecule should necessarily have permanent dipole moment.
 - Ex. HCl, CO, H_2O vapour, NO, etc.

Infra-red spectroscopy

- The light our eyes see is a small part of a broad spectrum of electromagnetic radiation.
- On the immediate high energy side of the visible spectrum lies the ultraviolet, and on the low energy side is the infrared.
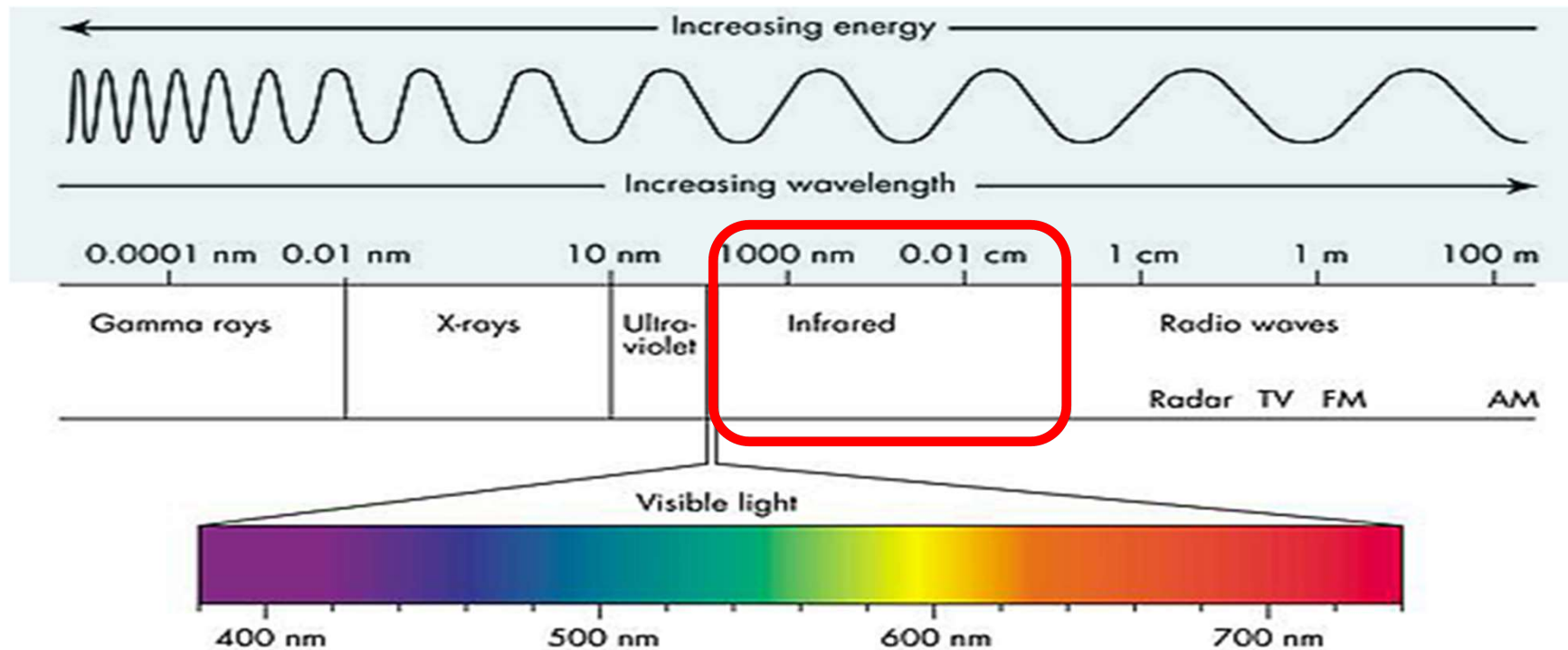
Infra-red spectroscopy

- The portion of the infrared region most useful for analysis of organic compounds is not immediately adjacent to the visible spectrum

	IR region	
Near IR	IR	Far IR
0.8-2.5 μ	2.5-15 μ	15-200 μ
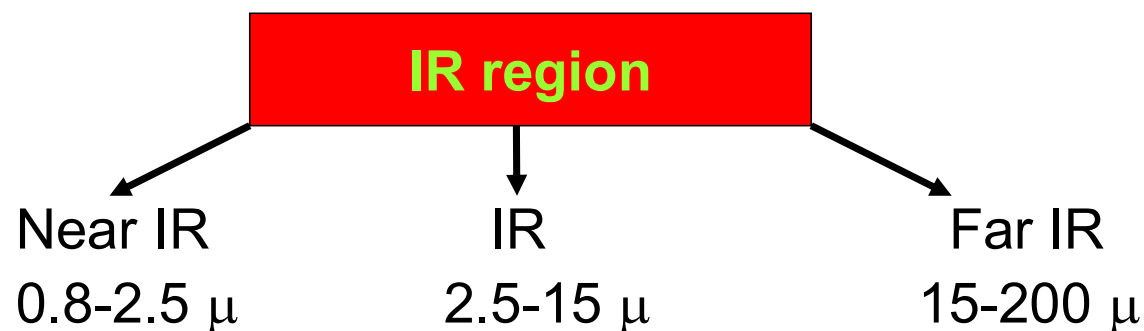
- Photon energies associated with infrared region are not large enough to excite electrons, but may induce vibrational excitation of covalently bonded atoms and groups.
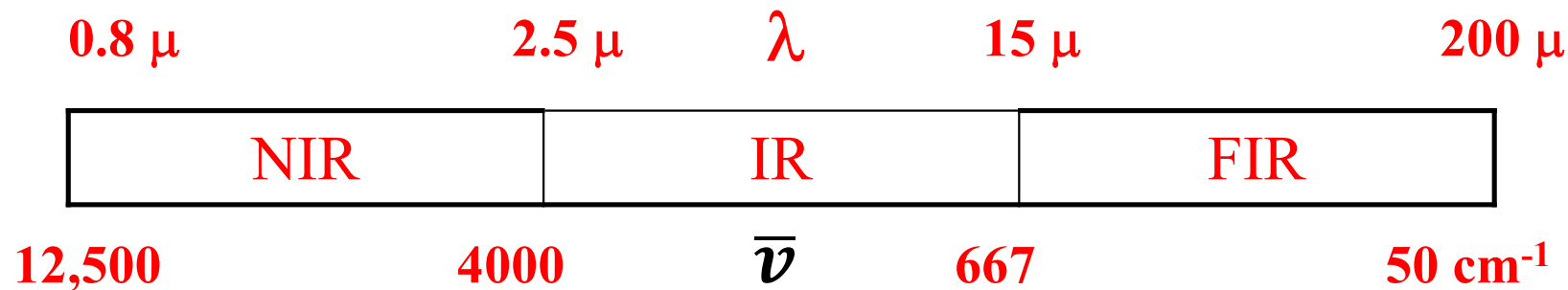
Infra-red spectroscopy

- Absorption of IR radiations can be expressed in terms of wavelength or wave number ($\bar{v}$) –*preferred*

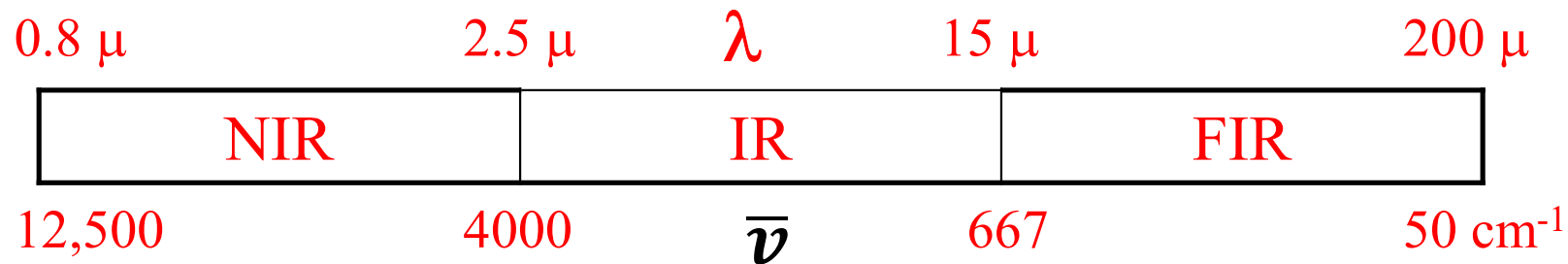$$\bar{v} \text{ in cm}^{-1} = \frac{1}{wavelength\ in\ cm}$$

for ex. λ = 15 μ = 15 x 10^{-4} cm

$$\bar{v} \text{ in cm}^{-1} = \frac{10000}{wavelength\ in\ \mu}$$

0.8 μ		2.5 μ	λ	15 μ		200 μ
	NIR		IR		FIR	
12,500		4000	$\overline{v}$	667		50 cm^{-1}

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Infra-red spectroscopy

0.8 μ		2.5 μ	λ	15 μ		200 μ
	NIR		IR		FIR	
12,500		4000	$\overline{v}$	667		50 cm^{-1}

Change in intensity

→ Absorbance (A)

$A = \log (1 / T)$

→ Transmittance (T) -*preferred*

- Infra-red spectra are plotted as percent transmittance (T) vs wave number ($\overline{v}$)

Infra-red spectroscopy

Source: https://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/Spectrpy/InfraRed/infrared.htm
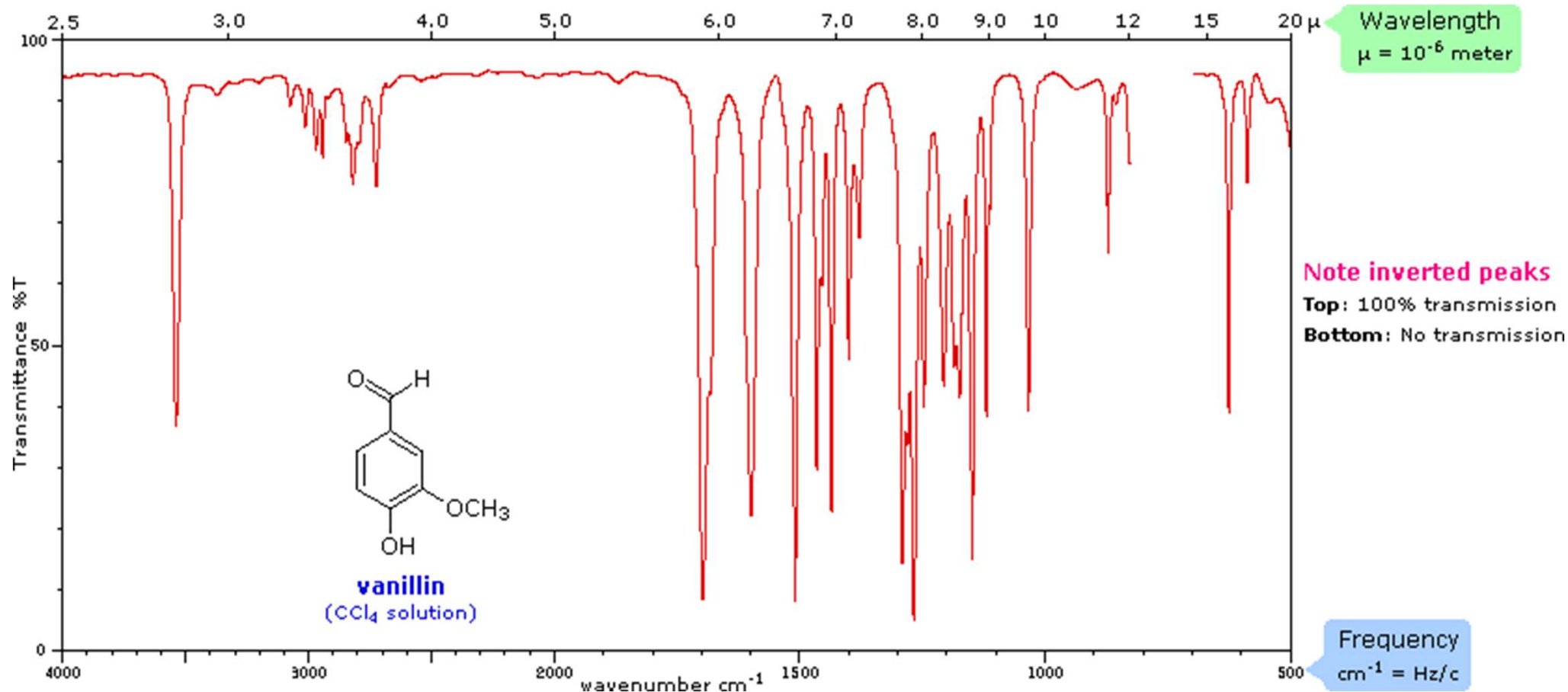
IR Spectra-vibrational transitions

- Vibrational rotational spectroscopy - Vibrational energy change is accompanied with large number of rotational energy changes.
- Vibrational energy levels - Quantized
- v – Vibrational quantum number i.e., 0,1,2,3,…….

  ν - Vibrational frequency

$$E_V = \left(v + \frac{1}{2}\right) h\nu$$

Lowest Vibrational level - $v = 0$,

$$E_V = \left(0 + \frac{1}{2}\right) h\nu = \frac{1}{2} h\nu : \text{Zero point energy}$$

$$E_1 = \frac{3}{2} h\nu \qquad\qquad E_2 = \frac{5}{2} h\nu \qquad\qquad E_3 = \frac{7}{2} h\nu$$

$$E_2 - E_1 = h\nu \qquad\qquad E_1 - E_0 = h\nu$$

IR Spectra-vibrational transitions

- Absorption of IR radiation equal to the energy difference between two vibrational levels cause a vibrational transition

- Transition from ground state (v = 0) to first excited state (v = 1) absorbs IR radiations strongly and gives rise to intense band called the **Fundamental Band.**

$$\Delta E_{vib} = \frac{3}{2} hv - \frac{1}{2} hv = hv$$

- Transition from ground state (v = 0) to second excited state (v = 2) gives rise to weak band called the **Overtone.**

$$\Delta E_{vib} = \frac{5}{2} hv - \frac{1}{2} hv = 2hv$$

IR Spectra-vibrational transitions

- All the vibrational energy levels are equally spaced by an spacing of $\mathbf{h}v$

$$\Delta v = \pm 1$$

$$\Delta v = +1 \ - \ \text{Operative part}$$

In the next session.....

- Molecular vibrations and Hooke's law