UCB008 - APPLIED CHEMISTRY

THAPAR INSTITUTE
OF ENGINEERING & TECHNOLOGY
(Deemed to be University)

SCBC-TIET

Molecular Spectroscopy Series

Lecture - II

Spectroscopy - Introduction

by

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Learning Outcomes

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

- Categorize molecular energy levels
- Illustrate types of molecular spectra
- Differentiate between atomic and molecular spectra

Molecular Energy Levels

- $E_{mol} = E_{el} + E_{vib} + E_{rot} + E_{tr}$

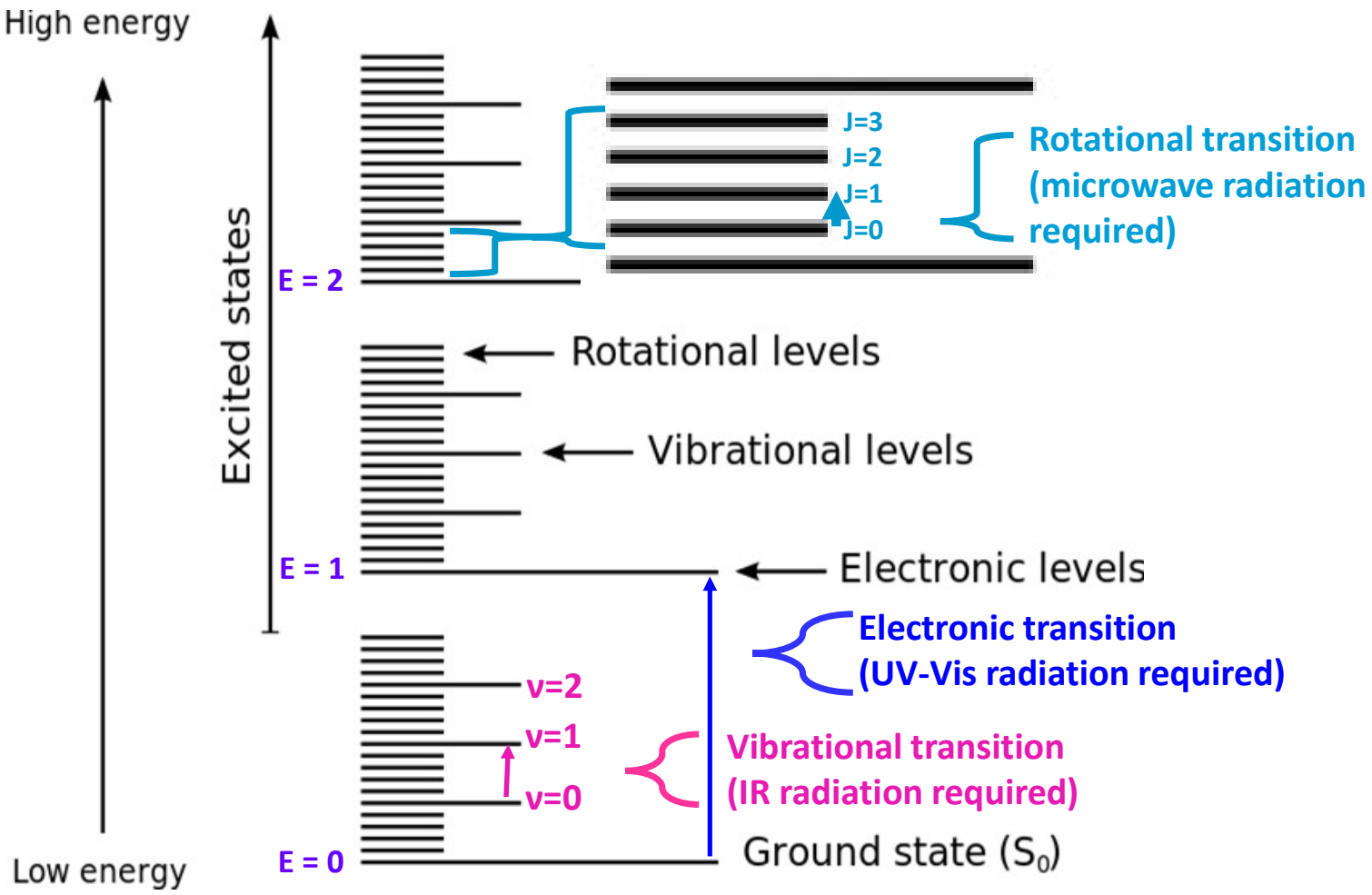
  $E_{el} >> E_{vib} > E_{rot} >> E_{tr}$ (E_{tr} is Negligible)

  $E_{mol} = E_{el} + E_{vib} + E_{rot}$

- Molecule – electronic, vibrational and rotational energy levels
- Energy requirement for transition - $E_{el} > E_{vib} > E_{rot}$

Energy levels in a molecule

$$\Delta E_{rotational} < \Delta E_{vibrational} < \Delta E_{electronic}$$



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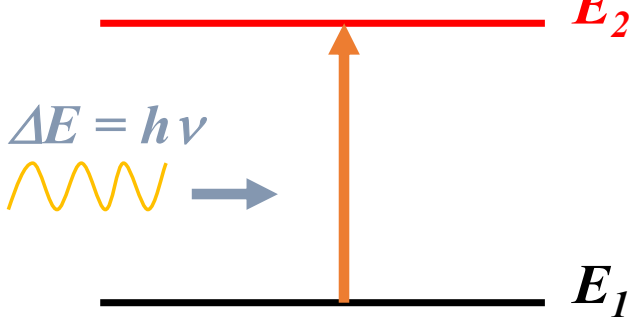
Spectroscopy

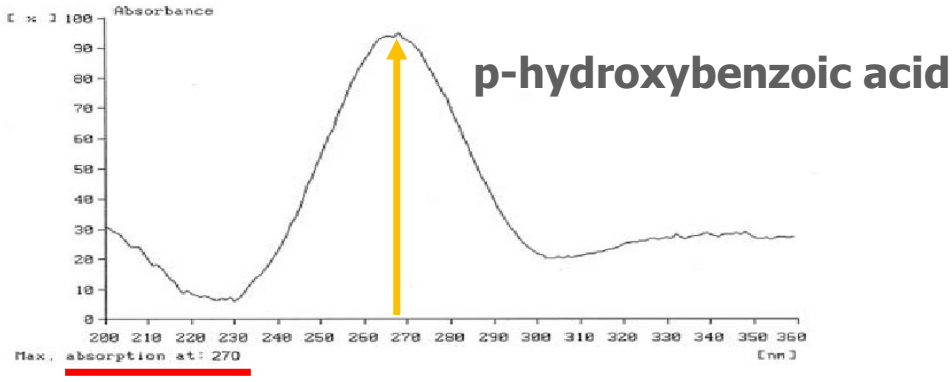
- Deals with the transitions that a molecule or an atom undergoes between its energy levels on the absorption of suitable radiation determined by quantum mechanical selection rules
- Spectrum is a graph of the intensity of absorbed or emitted radiation by sample verses frequency (ν) or wavelength (λ)
- Spectroscopy involves characterization of spectrum of a sample containing atoms or molecules
- The instrument used to obtain the spectrum of a compound is called a **Spectrometer/ Spectrophotometer**
- Spectra of a compound is highly characteristic, thus, spectroscopic techniques are used to determine the unknown molecular structures

Spectroscopy

1. Absorption Spectroscopy:

- Absorption spectroscopy is based on the measurement of absorption of electromagnetic radiation by atom or molecule.
- UV (185 - 380 nm) / Visible (380 - 760 nm) Spectroscopy, IR Spectroscopy

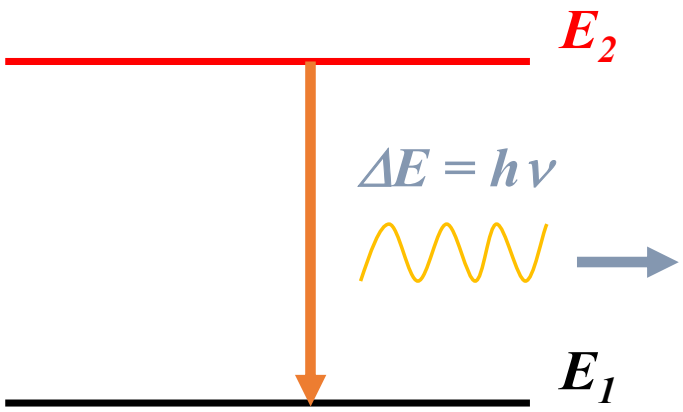


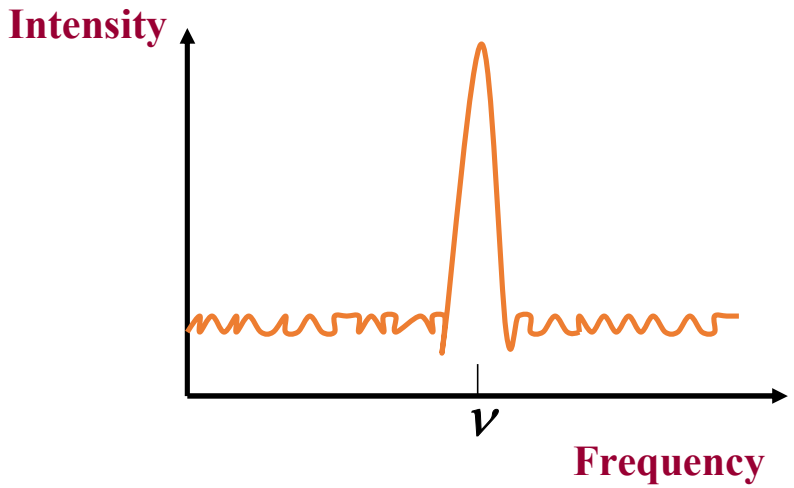


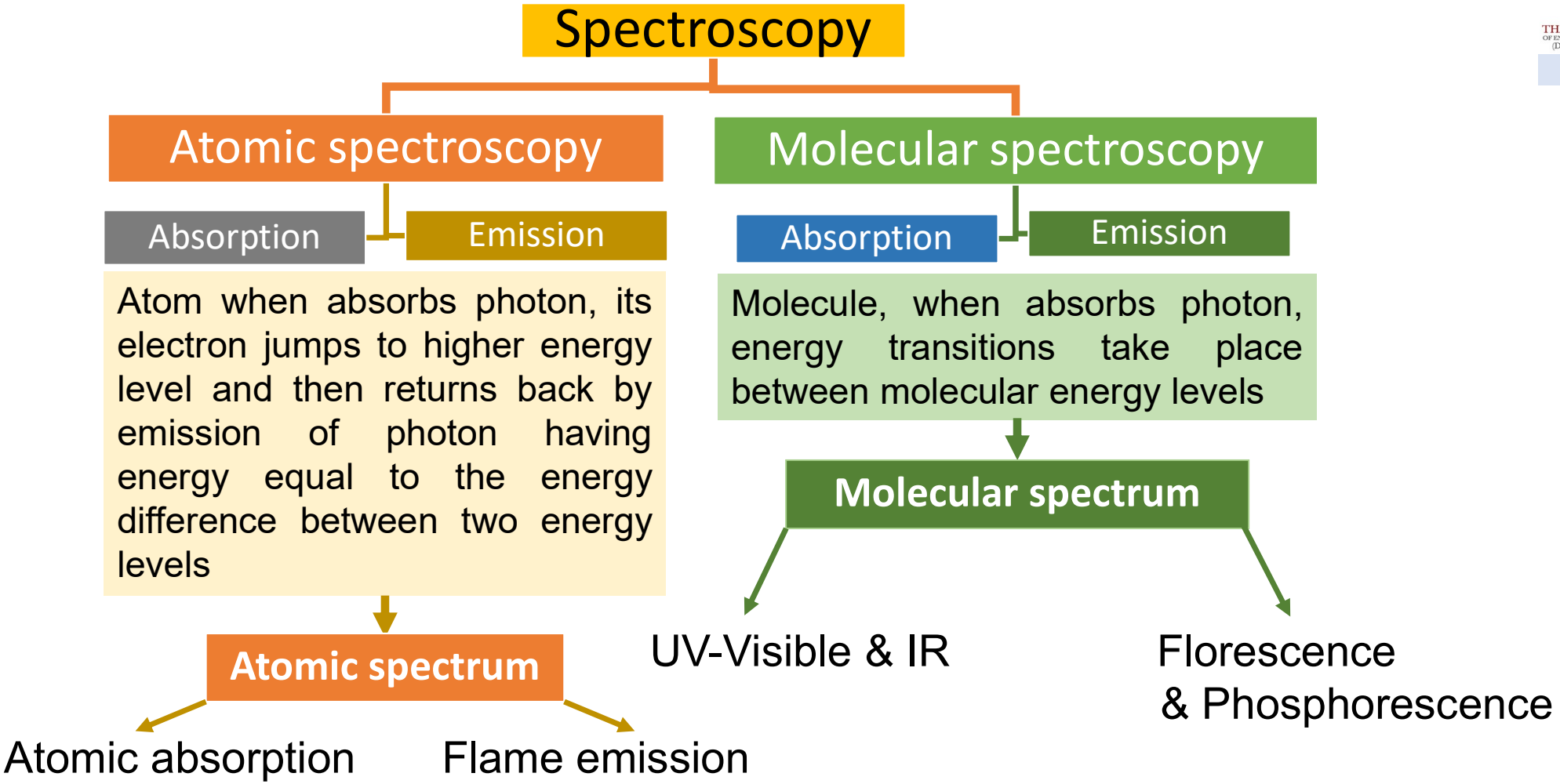
- λ_{max} – Wavelength at which a molecule shows maximum absorbance

Spectroscopy

2. Emission Spectroscopy:
   - Emitted radiations by atom or molecule are measured
   - Fluorescence, phosphorescence , etc.






Spectroscopy
Atomic spectroscopy
Molecular spectroscopy
Absorption
Emission
Absorption
Emission
Atom when absorbs photon, its electron jumps to higher energy level and then returns back by emission of photon having energy equal to the energy difference between two energy levels
Molecule, when absorbs photon, energy transitions take place between molecular energy levels
Molecular spectrum
Atomic spectrum
UV-Visible & IR
Florescence & Phosphorescence
Atomic absorption
Flame emission

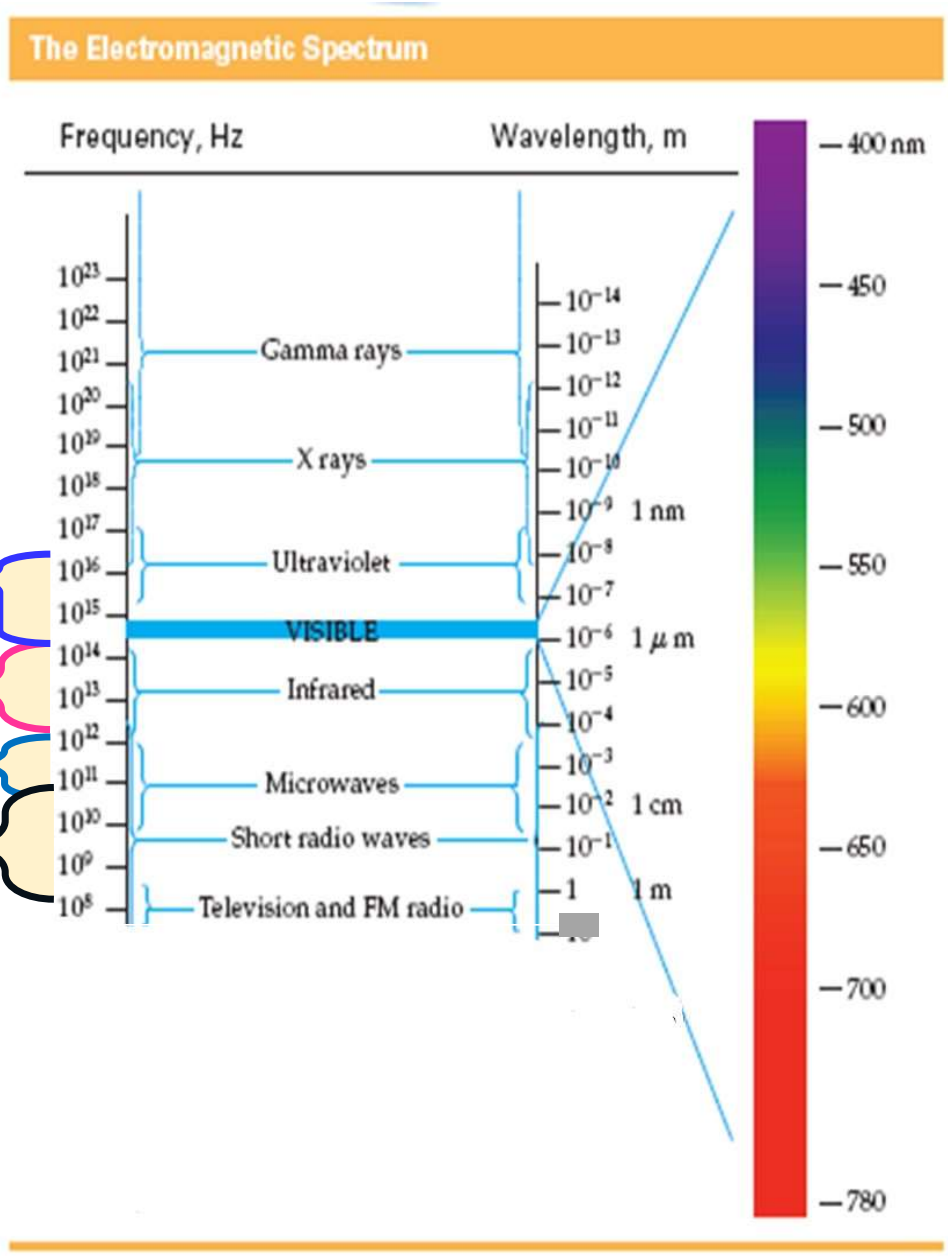
Types of Molecular spectra

Electronic or
UV-Vis. Spectra
(Electronic spectroscopy)

Vibrational spectra /
vibrational-Rotational
spectra / IR spectra
(IR/vibrational
spectroscopy)

Rotational Spectra
(Rotational/microwave
spectroscopy)
ESR spectra (ESR
spectroscopy)

NMR spectra
(NMR spectroscopy)



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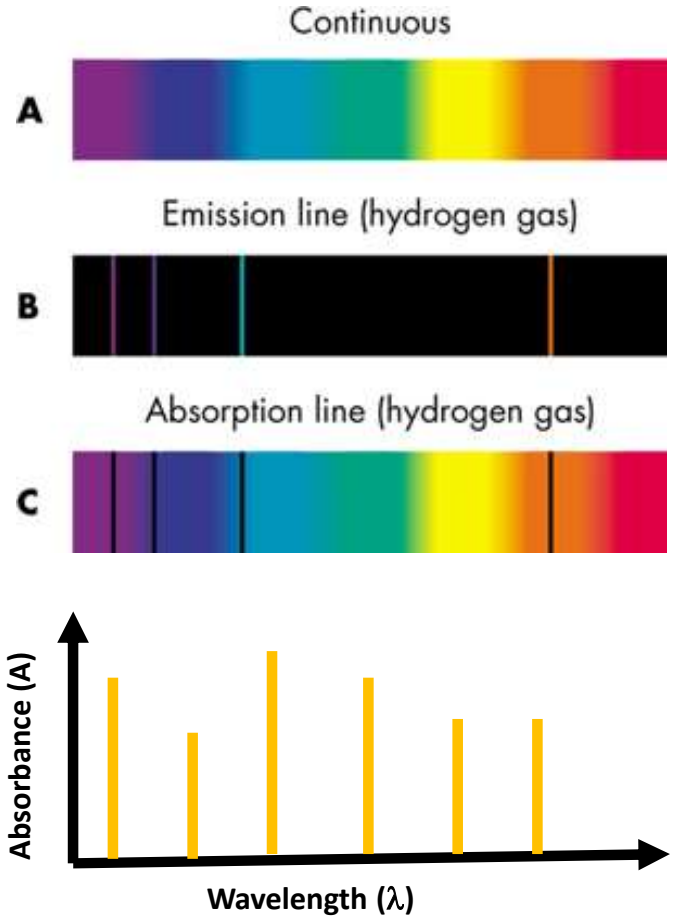
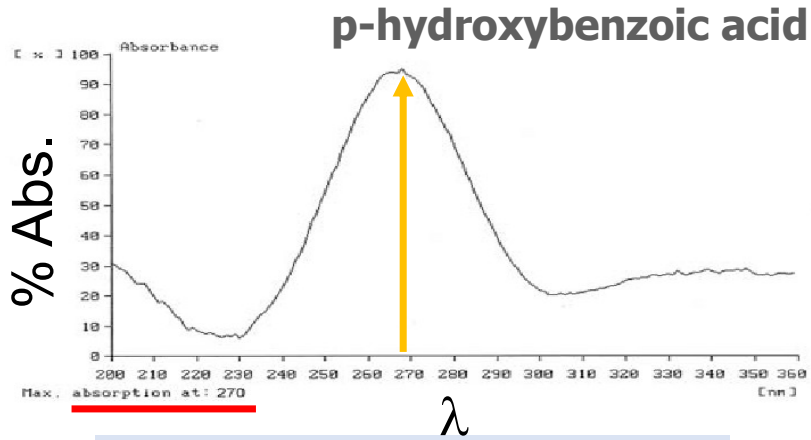
Atomic vs Molecular (Absorption) Spectrum - Difference



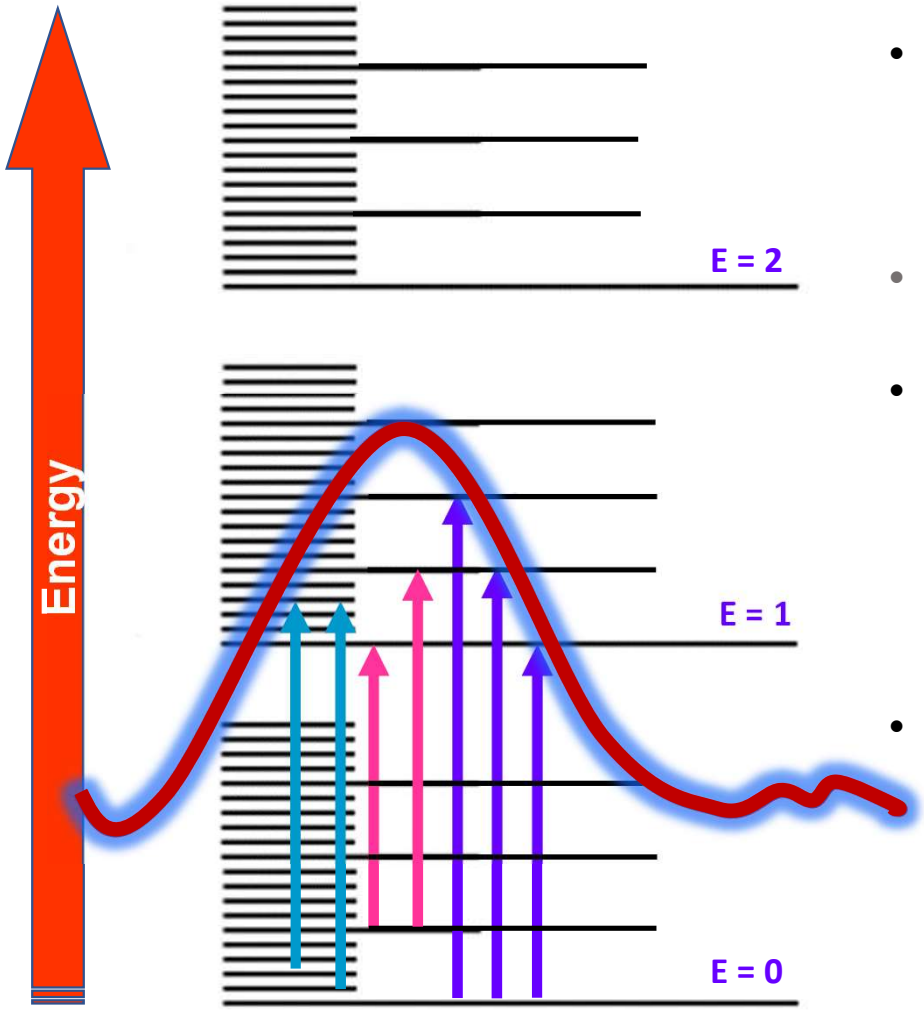
Atomic Absorption Spectrum

- **Atomic spectrum - Line spectrum**
- **Molecular spectrum – Band spectrum**



Molecular Absorption Spectrum

Atomic vs Molecular (Absorption) Spectrum - Difference



- Atoms have only electronic energy levels, whereas molecules have electronic, vibrational and rotational energy levels.
- Therefore, atoms have only electronic transitions **– Line spectrum**
- However, in case of molecule, electronic transitions are possible from any vibrational or rotational energy level of ground state to any vibrational or rotational energy level of excited state.
- Thus, vibrational and rotational effects get super imposed over electronic transition resulting in **an absorption band** instead of absorption lines

Spectroscopy

Molecule + EMR of suitable frequency

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Absorption of radiation

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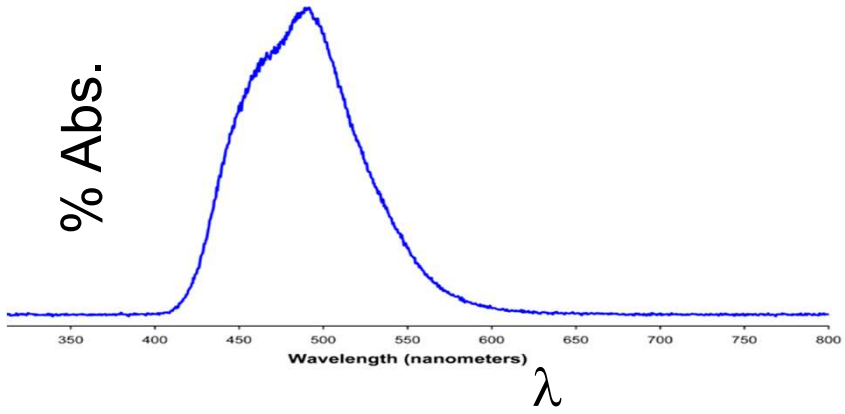
λ absorbed is measured by spectrophotometer

Changes in elec., vibrat. & rot. energy levels of the molecules



Highly characteristic of a molecule

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Technique is Used for structure determination

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In the next session.....

- Electronic transitions in the UV-visible spectroscopy