

# Molecular Spectroscopy



Online Workshop on Lectures and Virtual Practical Demonstrations, 6-19 July 2020

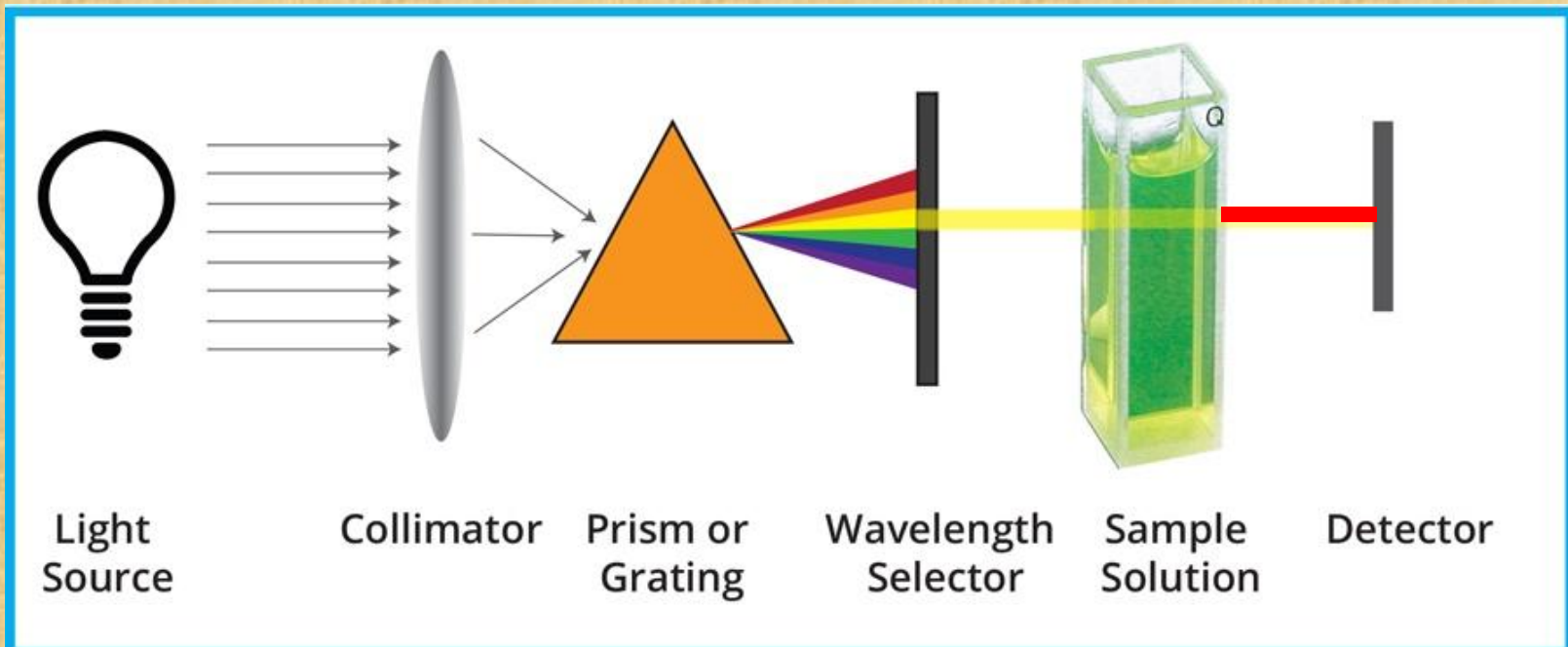
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Department of Physics and Materials Science & Engineering

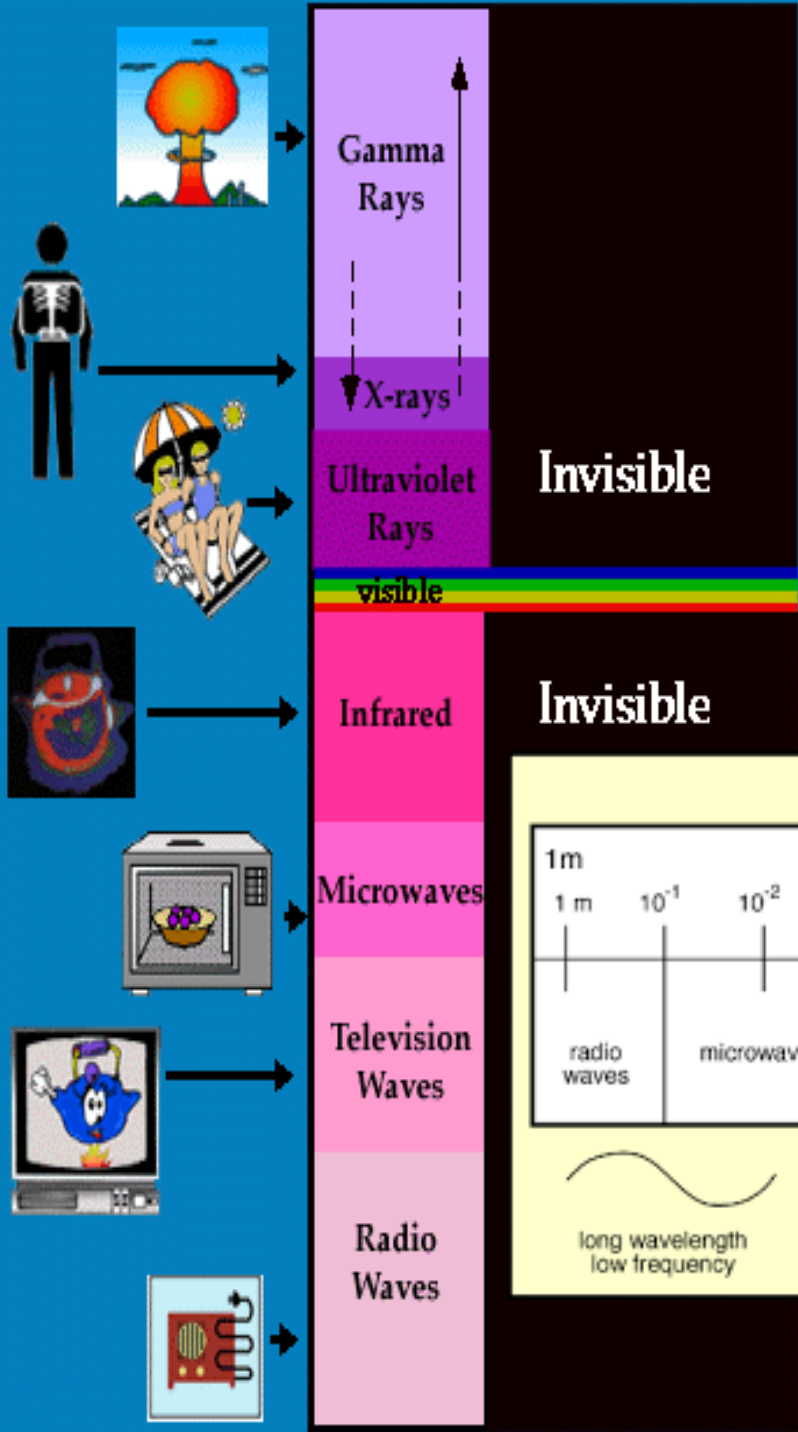
Jaypee Institute of Information Technology Noida, U.P.,  
India



- It is defined as the study of the interaction of electromagnetic radiation and matter.
- Due to interaction the incident of absorption or emission of electromagnetic radiation by the molecules happens.
- Output of the interaction provides data like frequency or wavelength of radiation and the intensity of radiation emitted or absorbed by the molecule.
- In this way we can determine the size, shape, flexibility, electronic arrangement of the molecule means molecule structure studies.

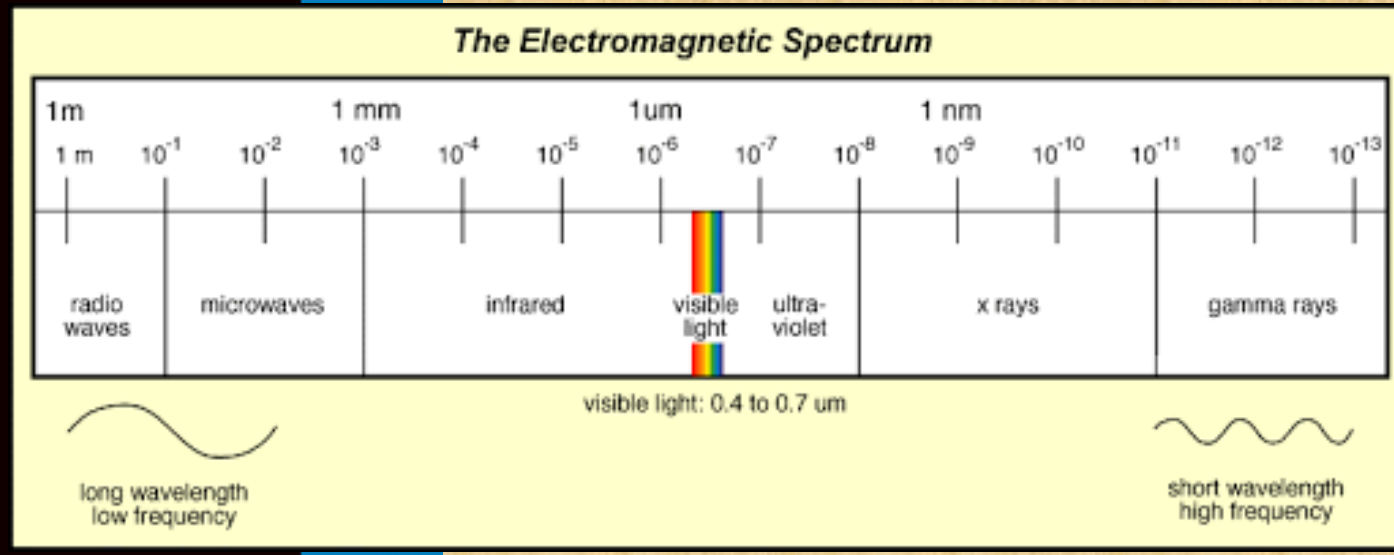
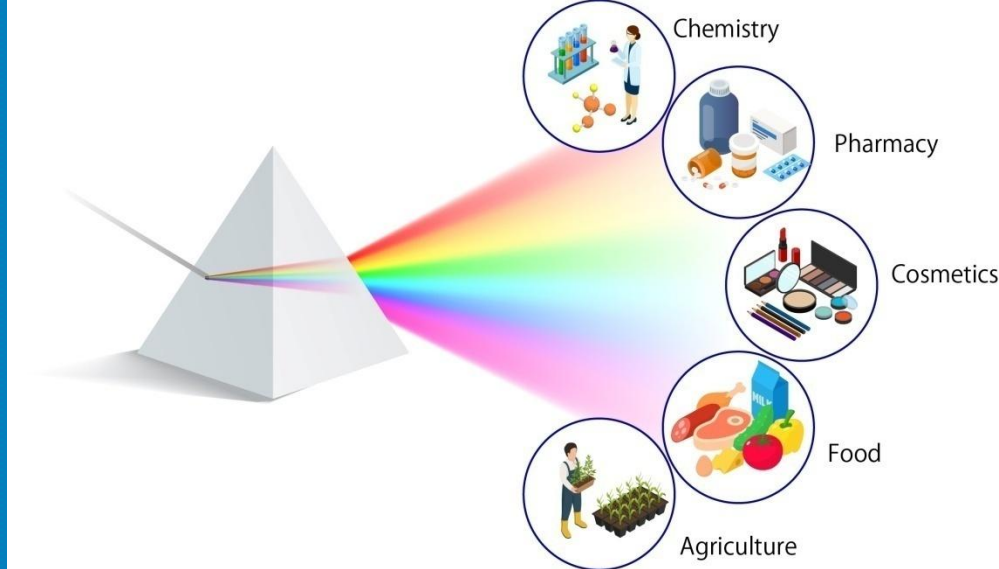






**Invisible**

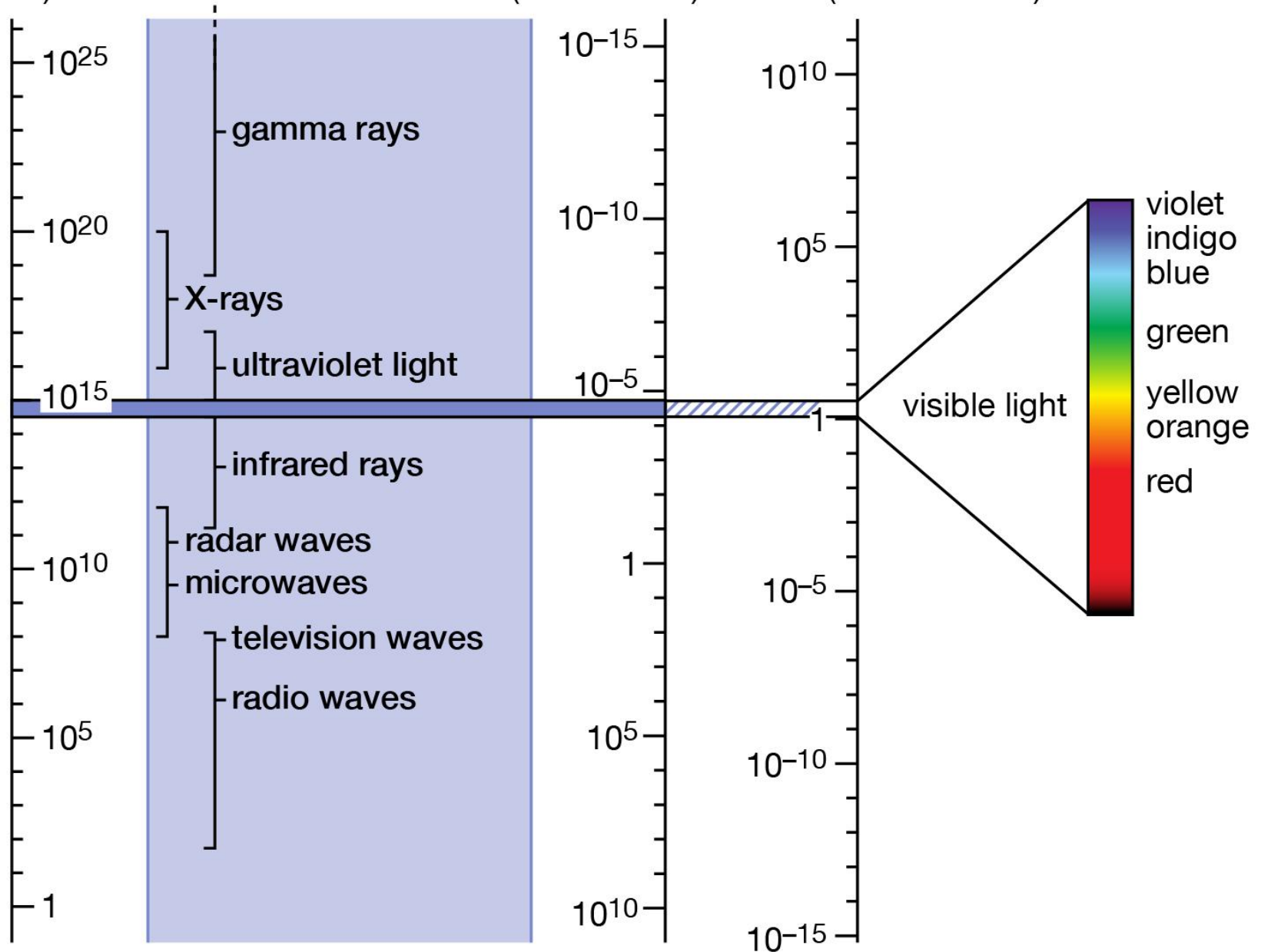
**Invisible**



frequency  
 $\nu$  (hertz)

wavelength  
 $\lambda$  (centimetres)

photon energy  
 $h\nu$  (electron volts)



# Different kind of spectroscopy

- **Microwave Spectroscopy.**
- **Infrared Spectroscopy.**
- **Raman Spectroscopy**
- **Electronic Spectroscopy**
- **Spin Resonance ( NMR and ESR Spectroscopy)**
- **X-ray Crystallography**
- **Mass Spectroscopy**
- **Electron Microscopy**

## **APPLICATIONS**

*Depending upon the frequency range they are classified. Each class has its unique set of application in Physics, Chemistry, Biology, Electronics, Biotechnology and other fields.*

## The main characteristics of Electromagnetic Radiation:

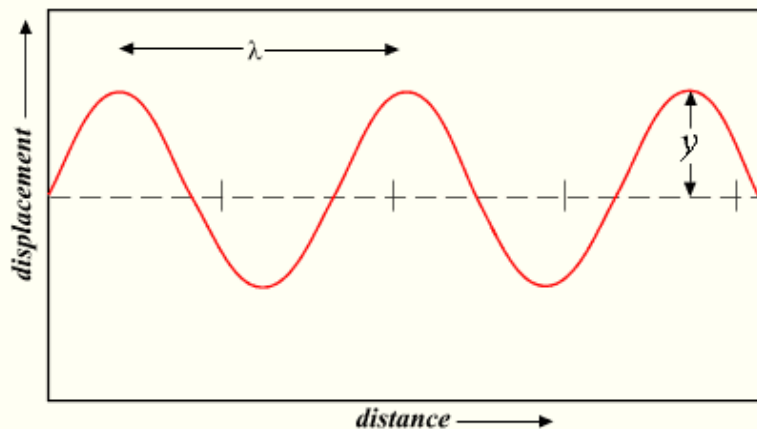
- $\lambda$  - wavelength of light
- $c$  - Velocity (distance travelled per second)  $3 \times 10^{10}$  cm/sec
- $\nu$  - Frequency – (Number of waves per second)  $= c/\lambda$
- $\bar{\nu}$  - Wave number = Number of waves per centimeter  
 $= \nu/c = 1/\lambda$
- $E$  – Energy
- $E = h\nu$ , Plank's Law =  $h/2\pi \cdot 2\pi\nu = \hbar \omega$
- $\omega$  = angular velocity (angle subtended per second)



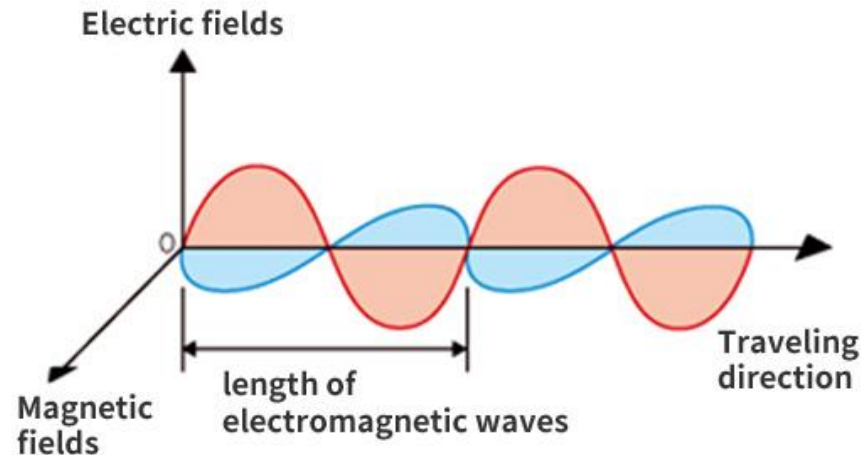
# Wavelength, frequency and energy of radiation

- Electronic radiation may be considered as a simple harmonic wave propagated from a source and travelling in straight lines.
- Electromagnetic radiation associates electric and magnetic fields where both fields are perpendicular to each other and to the direction of propagation.

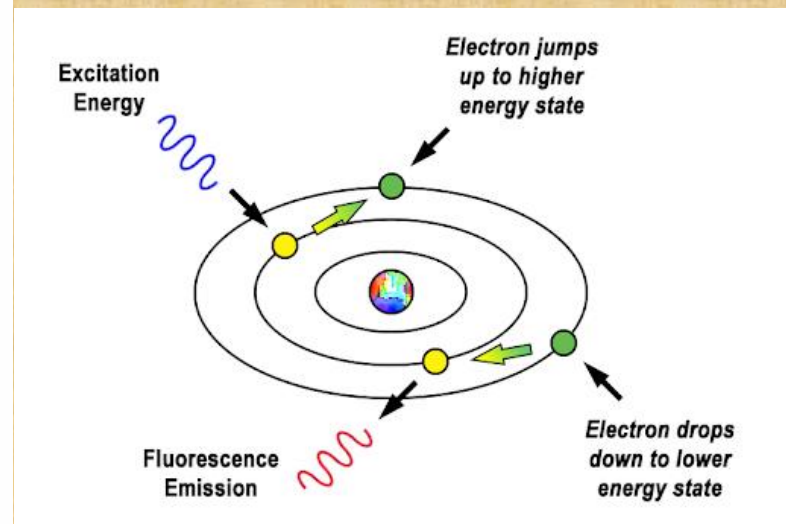
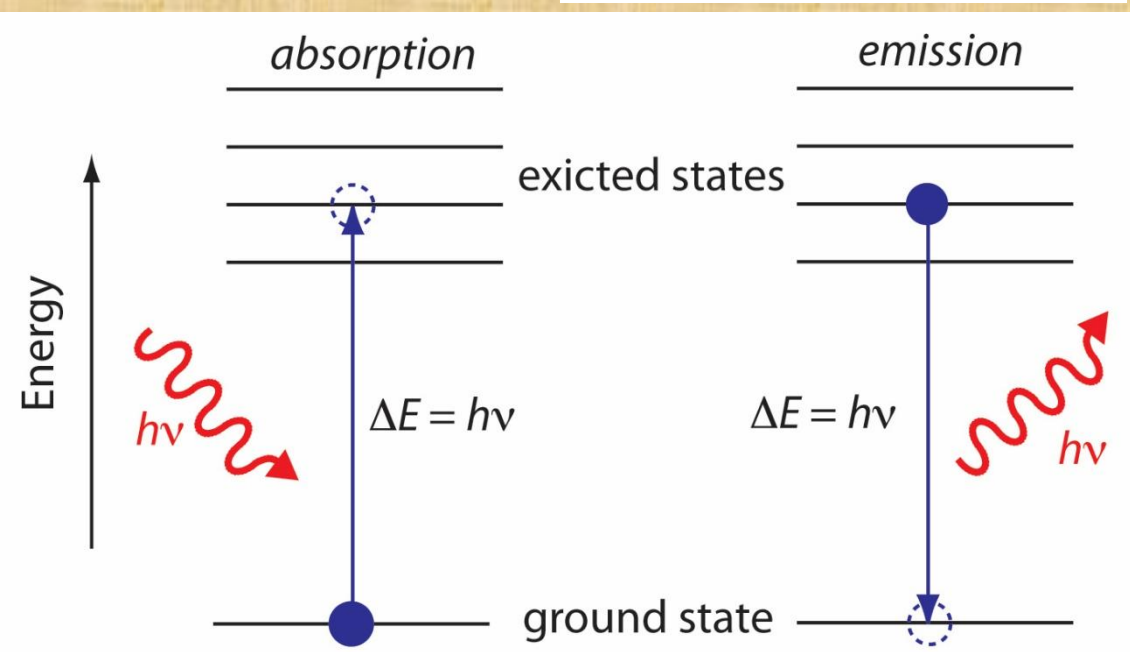
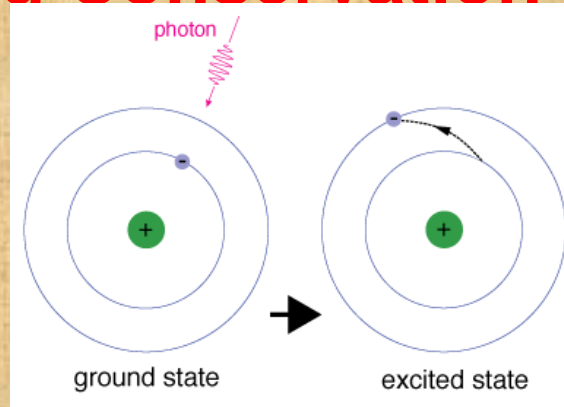
Wave



$\lambda = \text{wavelength}$   
 $y = \text{amplitude}$



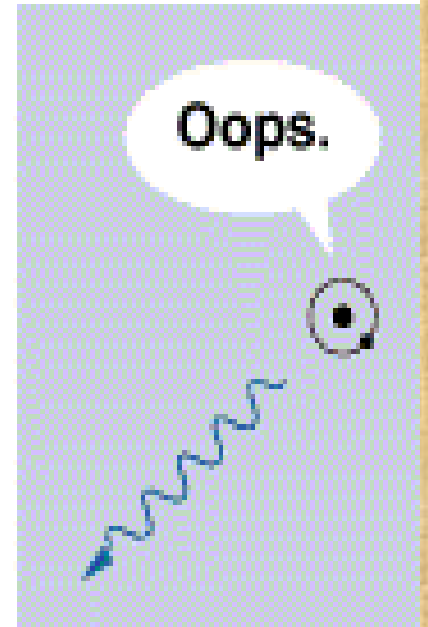
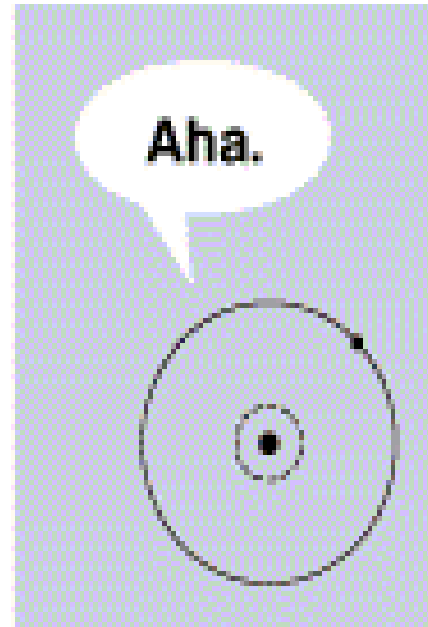
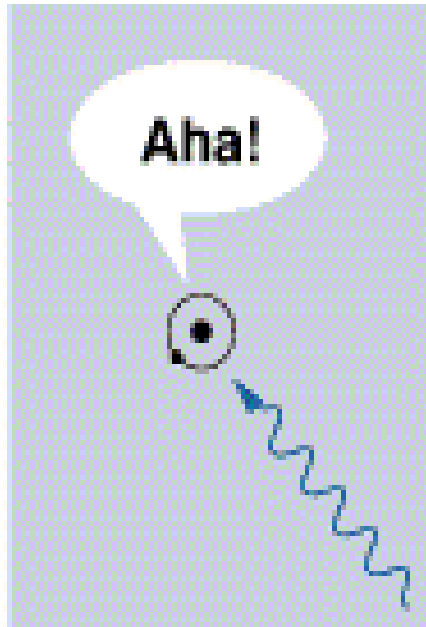
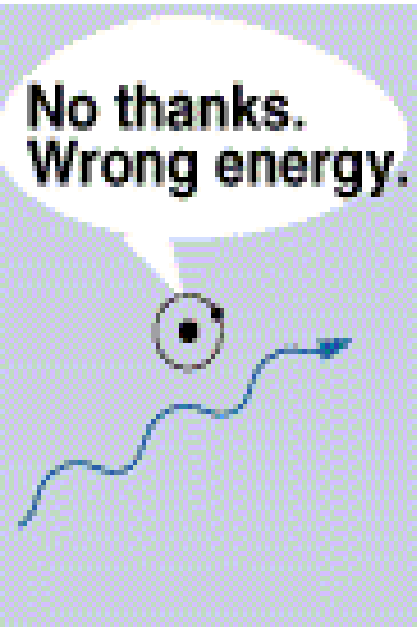
# Absorption / Emission of Photons and Conservation of Energy



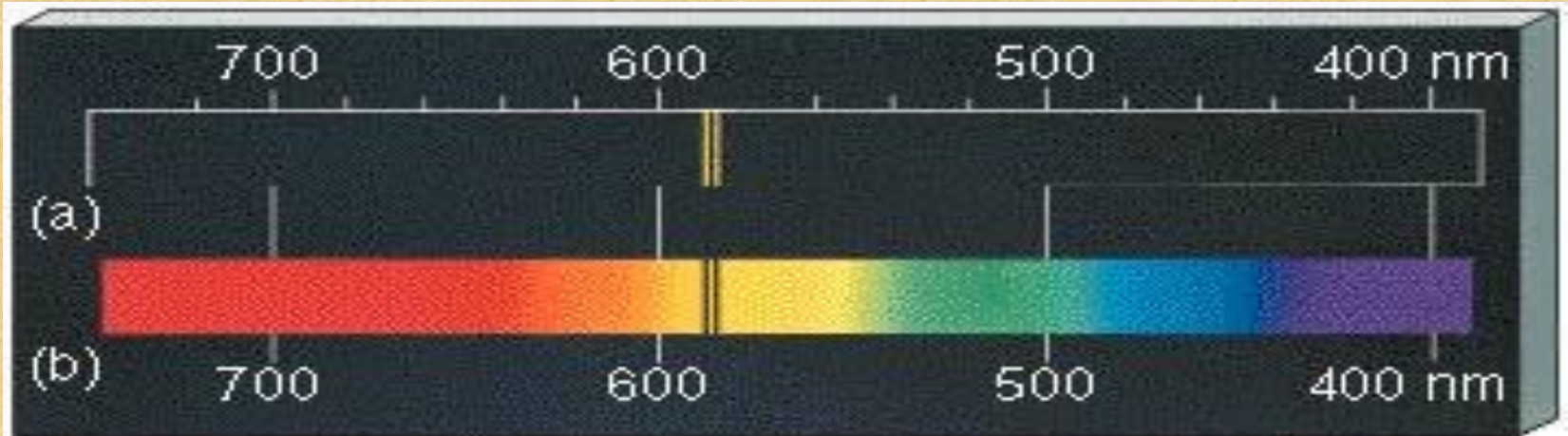
$$E_g - E_e = \Delta E = h\nu \quad E_e - E_g = h\nu$$



# Absorption vs. Emission

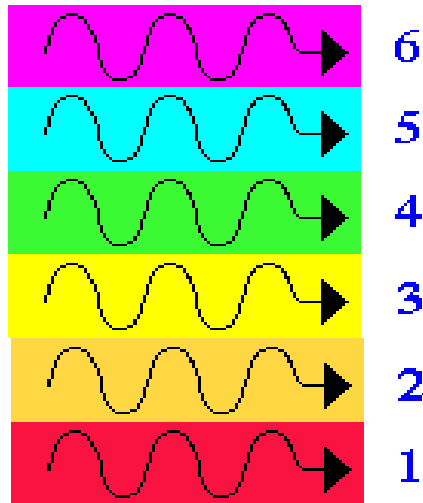


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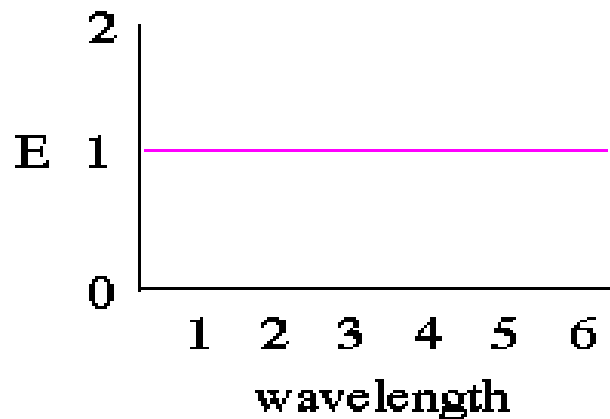


# Understanding emission and absorption

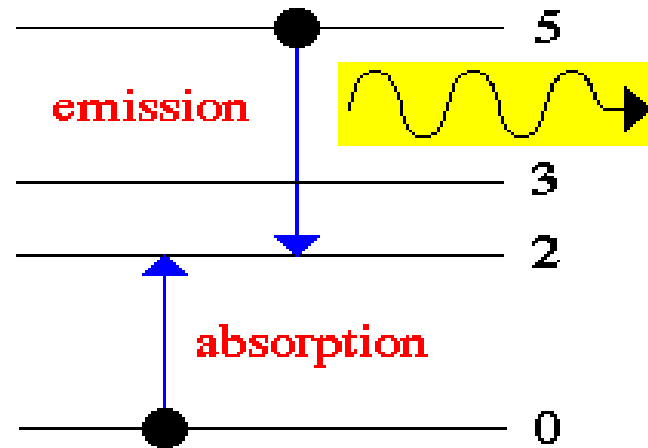
photons (energy)



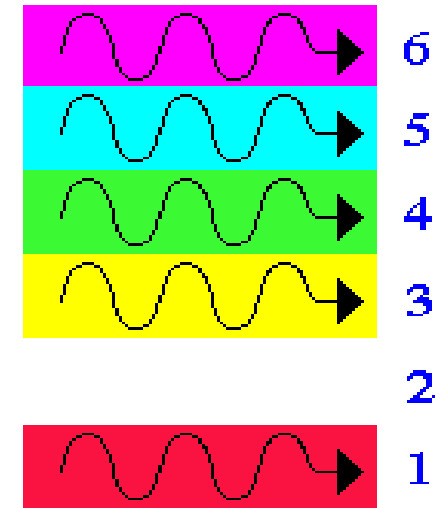
before spectrum



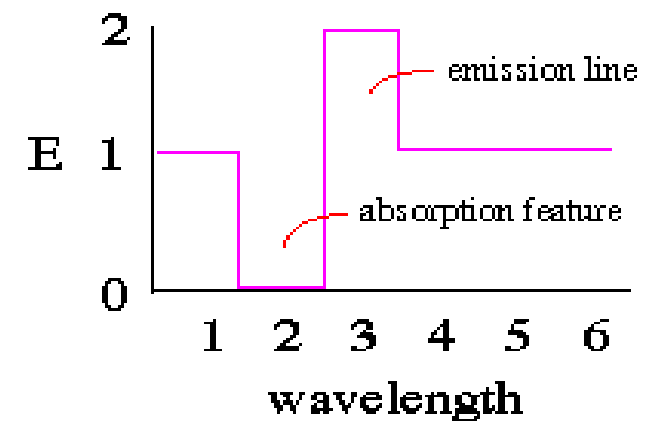
energy level



Bohr atom

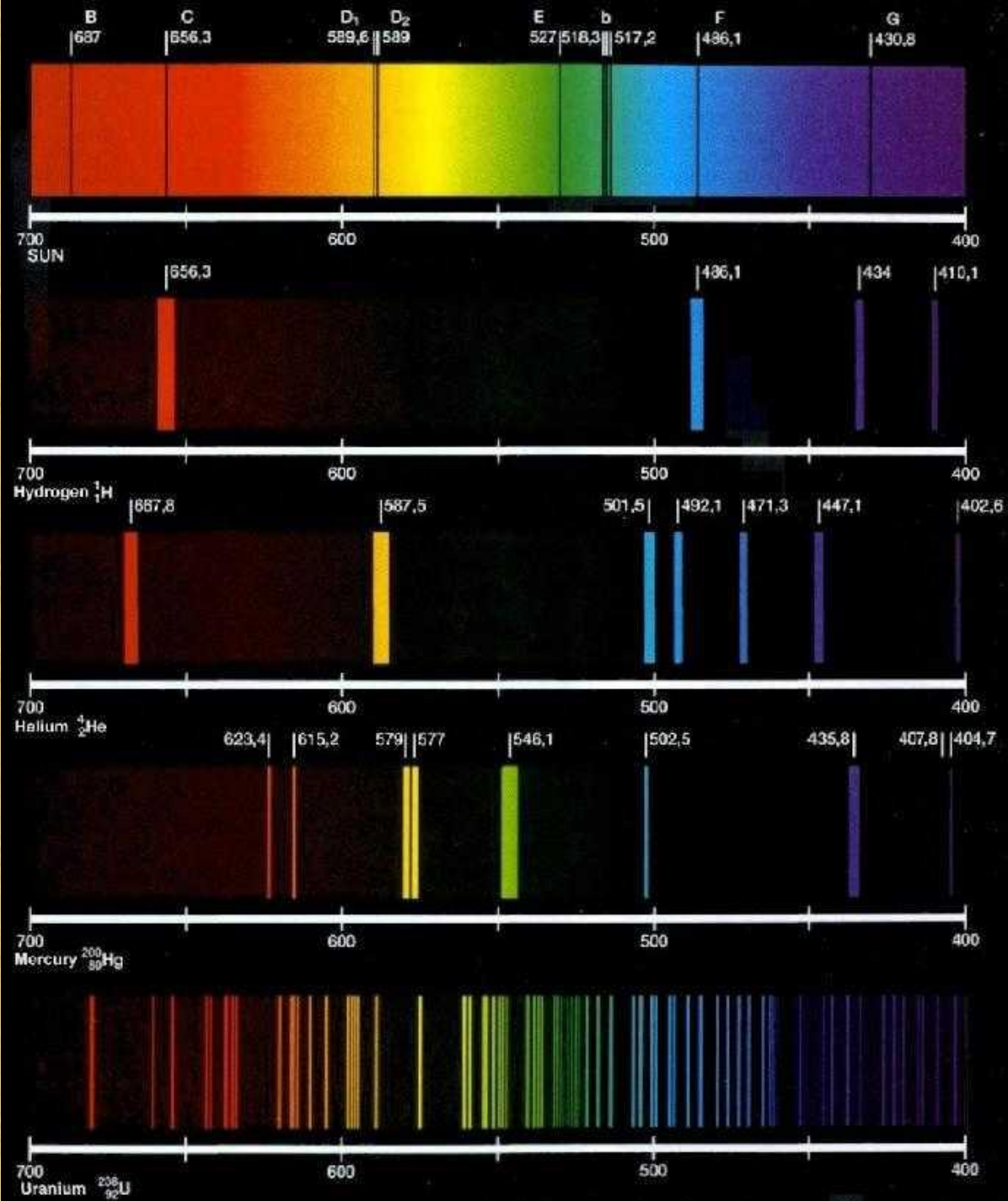


after spectrum



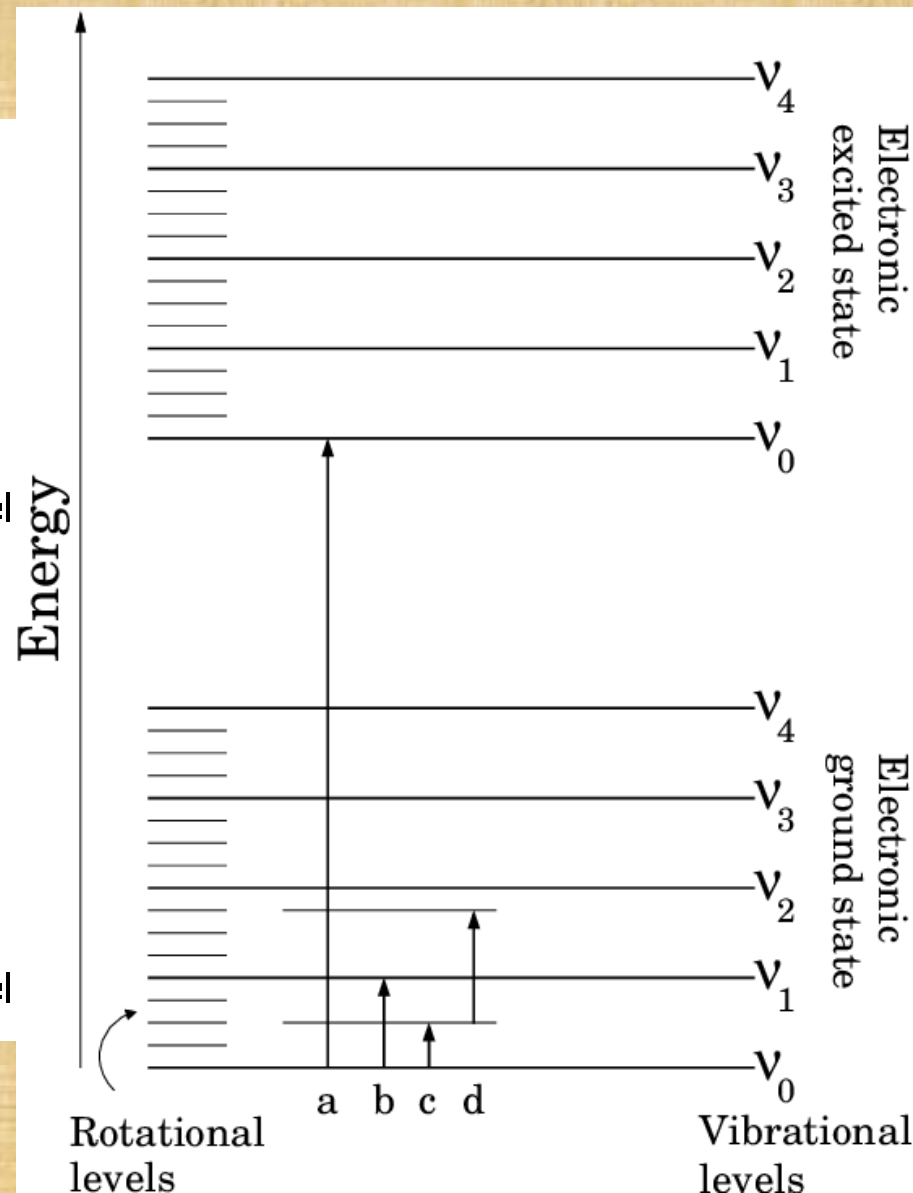
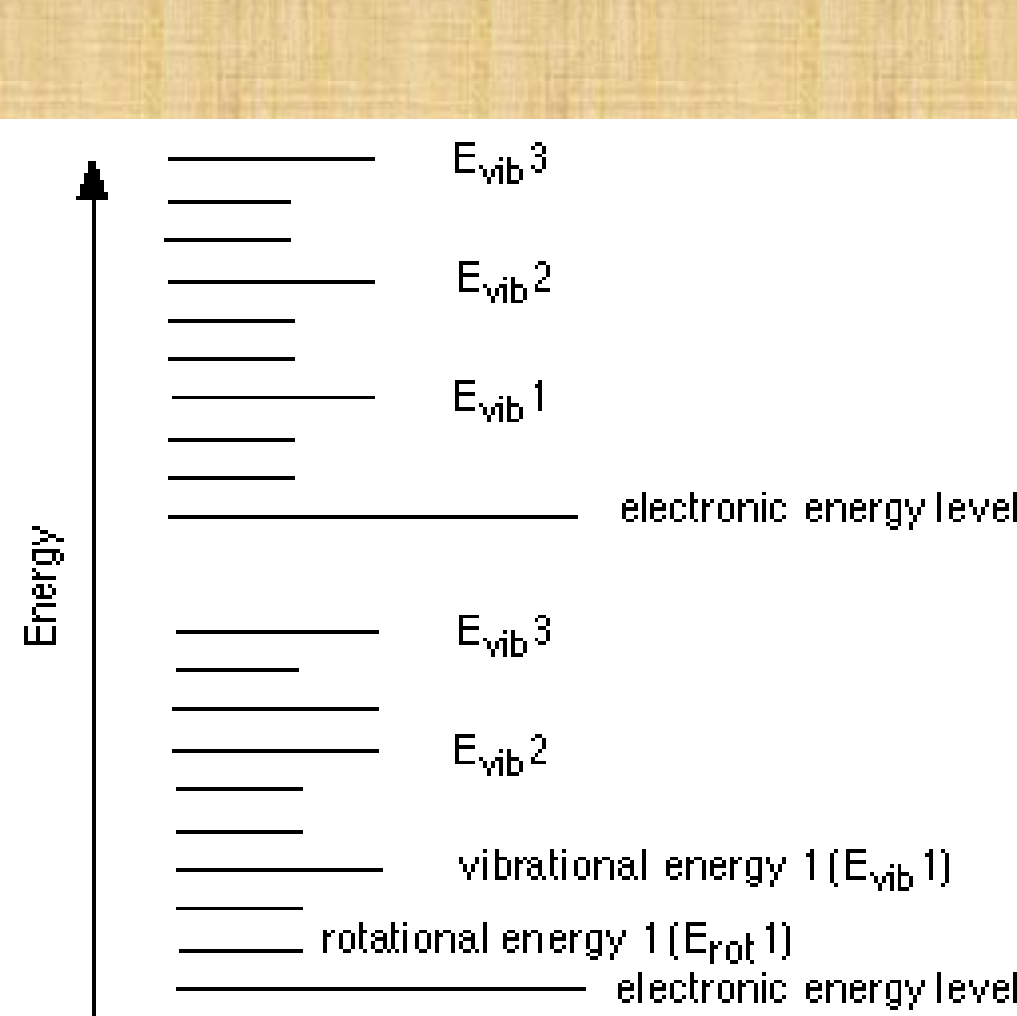
Absorption spectrum of Sun

Emission spectra of various elements



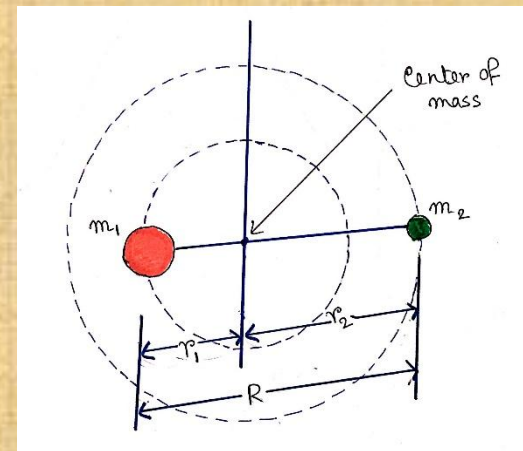


# Energy levels of a molecule

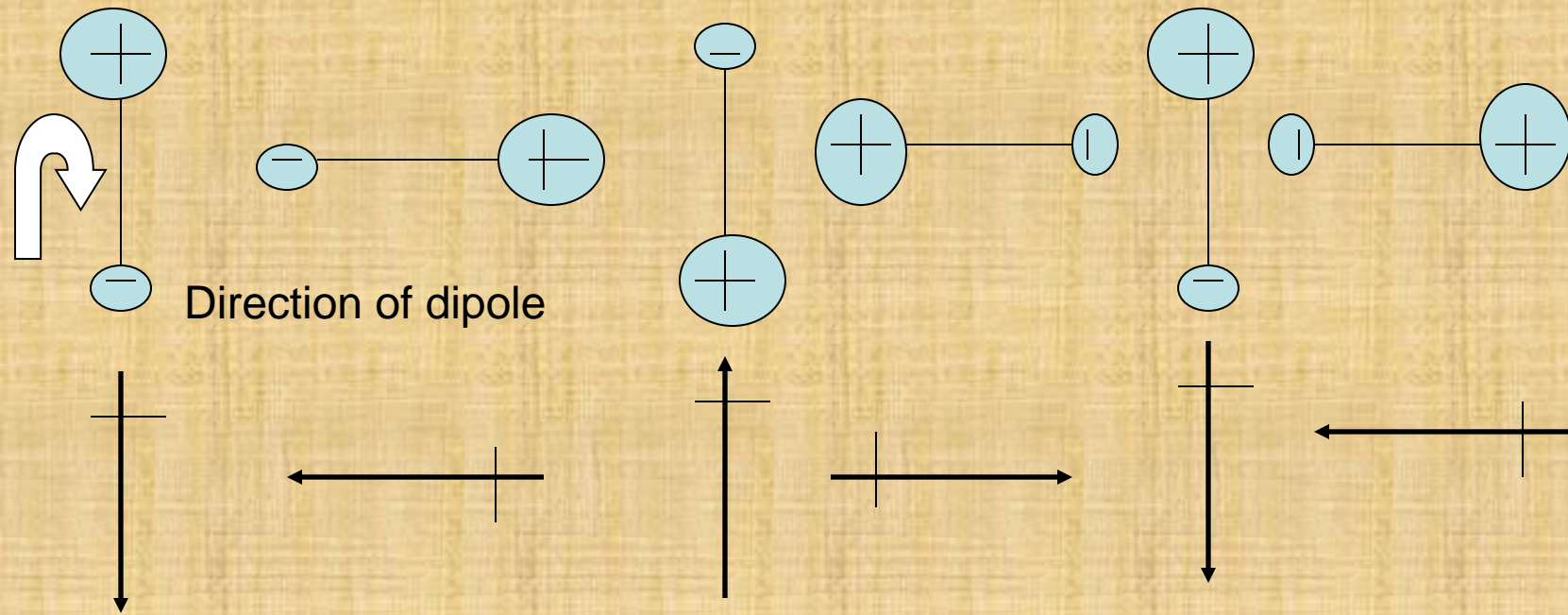


# Microwave region in electromagnetic spectrum

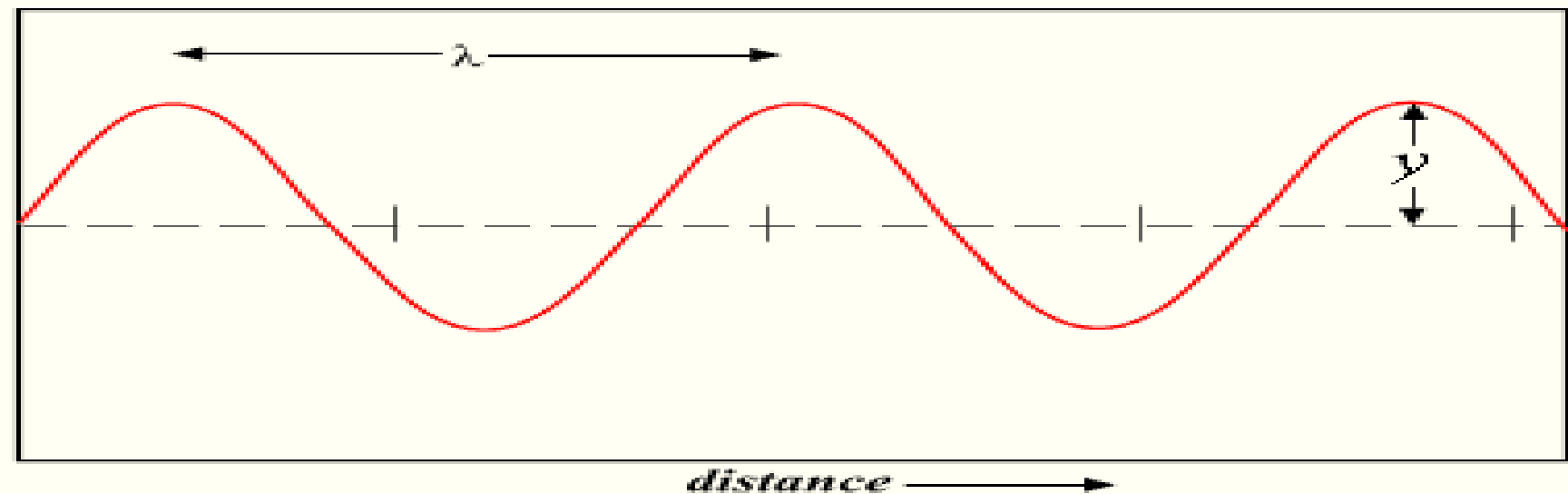
- Change in orientation
- Wave number =  $1-100 \text{ cm}^{-1}$
- Wavelength =  $1 \text{ cm} - 100 \mu\text{m}$
- Frequency =  $3 \times 10^{10} - 3 \times 10^{12} \text{ Hz}$
- Energy =  $10 - 10^3 \text{ Joules/mole}$



# DIRECTION OF ORIENTATION

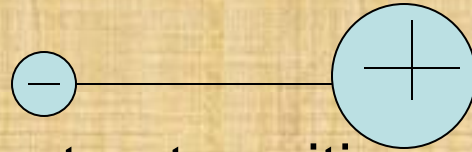


## *Wave*

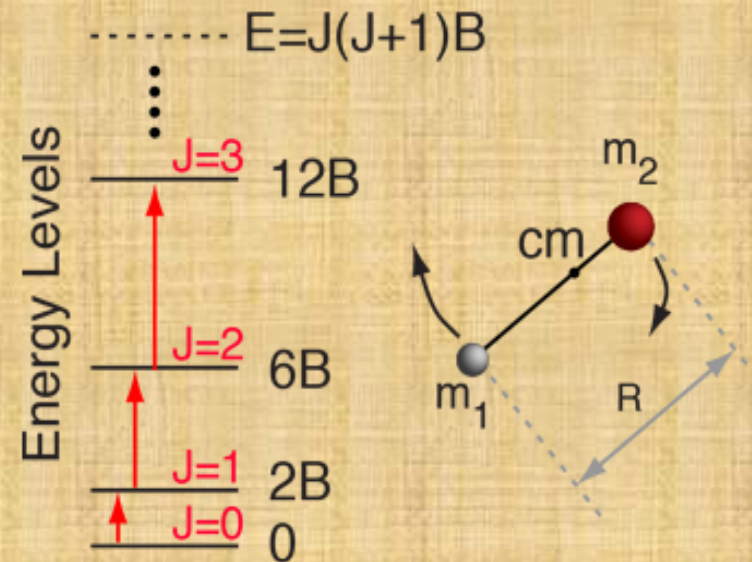




- The molecules which shows microwave spectra must carry permanent electric dipole moment.



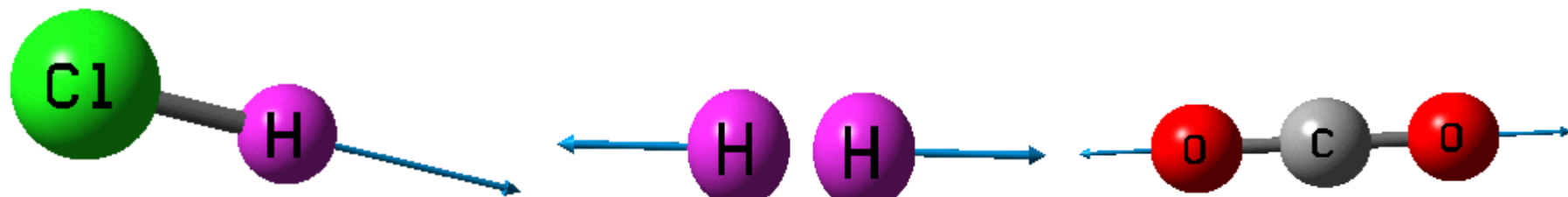
- Carries a permanent net positive charge and other a net negative charge.
- The rotation of this type of molecule with center of gravity remain fixed.
- All molecules having permanent moment are microwave active. HCl, HBr etc.



# Infrared/Vibrational Spectroscopy

# Vibrational (Infrared) spectrum

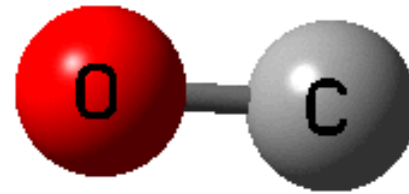
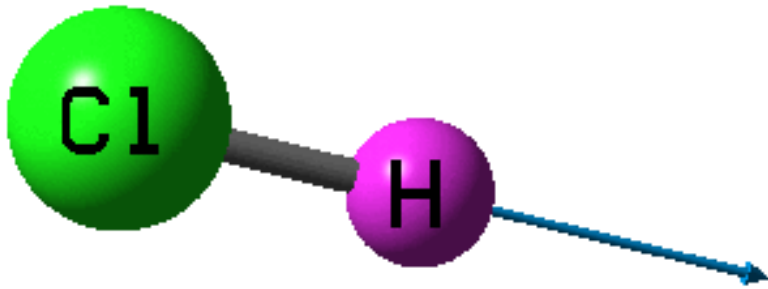
- If the relative displacement of a molecular vibration about their mean position gives rise a dipole change along the direction of displacement during the vibration, molecule shows vibrational spectrum.



- In order to be infrared active , there must be a dipole change during the vibration and this change may take place either along the line of symmetry axis or perpendicular to it



•Vibrational spectra will be observable only in heteronuclear molecules since homonuclear molecules have no dipole moment



•If the atom is removed a distance from its equilibrium position, it experiences a restoring force that is proportional to its displacement from the equilibrium position. The molecule then behaves like a spring.

- The spring which behaves in this manner is said to obey Hooke's law:

$$f \propto x$$

$$\Rightarrow f = -kx$$

- $x$  is the measure of the displacement from the equilibrium position,  $f$  is the force which the spring imposes on atom.  $k$  is a proportionality constant called the force constant, it gives the restoring force from equilibrium position.

- Negative sign is due to as  $x$  increases in one direction the force increases in opposite direction.
- Hook's law implies that the energy of the particle increases as the particle moves in either direction.
- Let work that must be done to displace the particle a distance  $dx$  is  $f_{\text{applied}} dx$ , and this work is stored as potential energy  $U$ . Thus

$$dU = f_{\text{applied}} dx$$

- Force  $f$  that the spring exerts on the particle and it acts against the applied force as  $f = - f_{\text{applied}}$

$$dU = (-f) dx$$

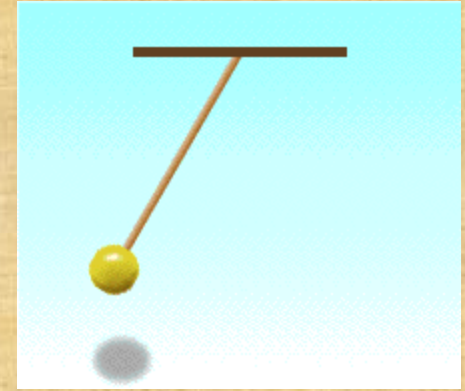
This is an important Relation between force And potential energy.

$$\Rightarrow \frac{dU}{dx} = -f$$

$$f = -kx$$

$$\frac{dU}{dx} = kx \Rightarrow dU = kx dx$$

$$\Rightarrow U = \frac{1}{2} kx^2$$



If after stretching length of the string is  $r$  and equilibrium Length is  $r_e$  then

$$f = -k(r - r_e) \quad \text{and} \quad U = \frac{1}{2} k(r - r_e)^2$$

If we want to describe the motion of the particle then we may use Newton's law as  $f = ma$  as

$$-kx = m \frac{d^2 x}{dt^2} \Rightarrow -kx = m \ddot{x}$$

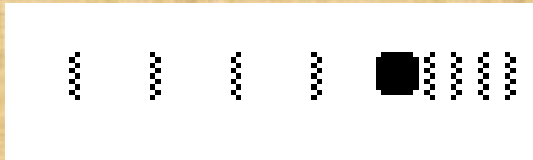


this equation has the solution of the form

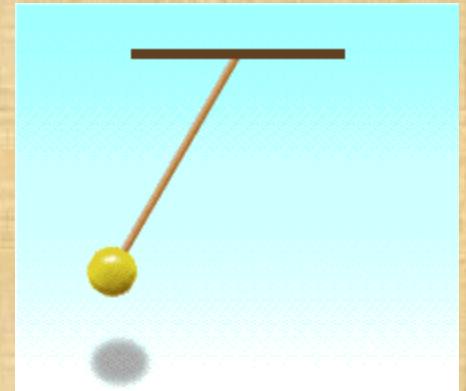
$$x = A \cos(2\pi\omega t + \varphi)$$

The correctness of this solution can be verified by substituting This and its second derivative back into the differential equ. When this is done one obtain an equality if

$$-4\pi^2\omega^2 m = -k$$



$$\Rightarrow \omega = \frac{1}{2\pi} \sqrt{\frac{k}{m}} \text{ Hz}$$



$$\bar{\omega} = \frac{1}{2\pi c} \sqrt{\frac{k}{m}} \text{ cm}^{-1}$$

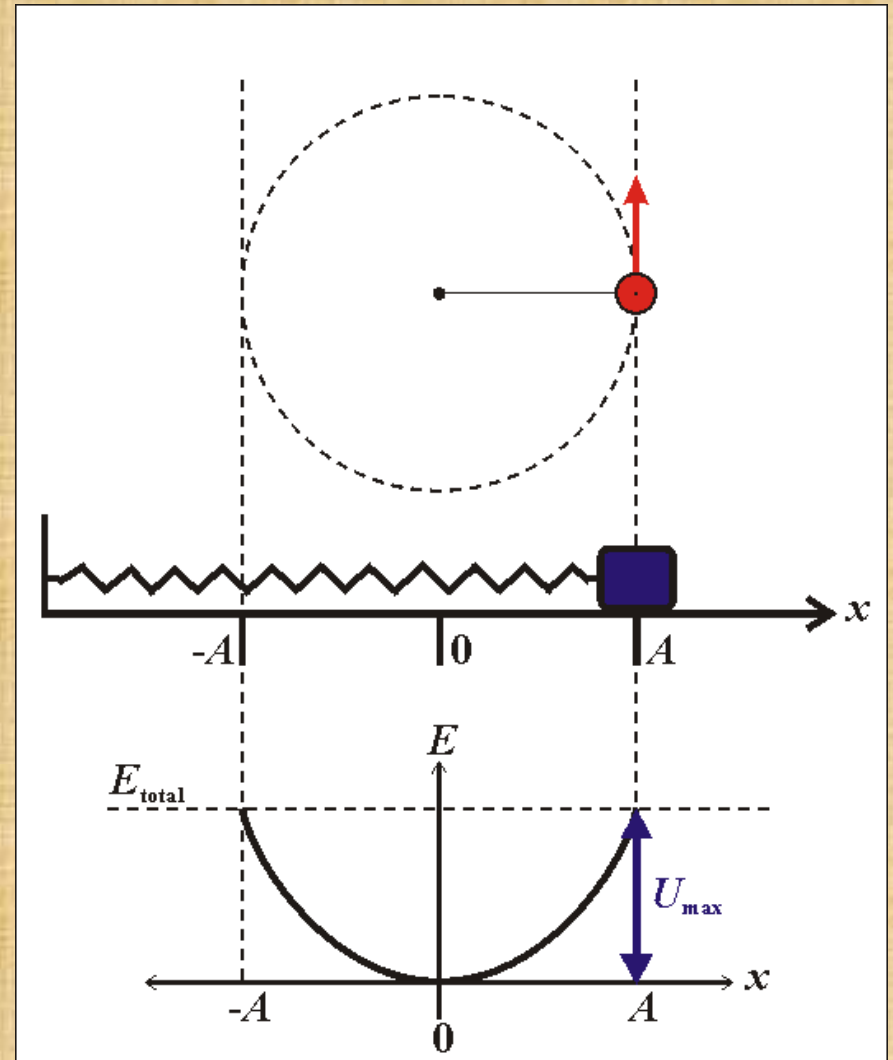
This shows that a particle with mass  $m$  held by a spring with Force constant  $k$  will vibrate with frequency  $\omega$ .

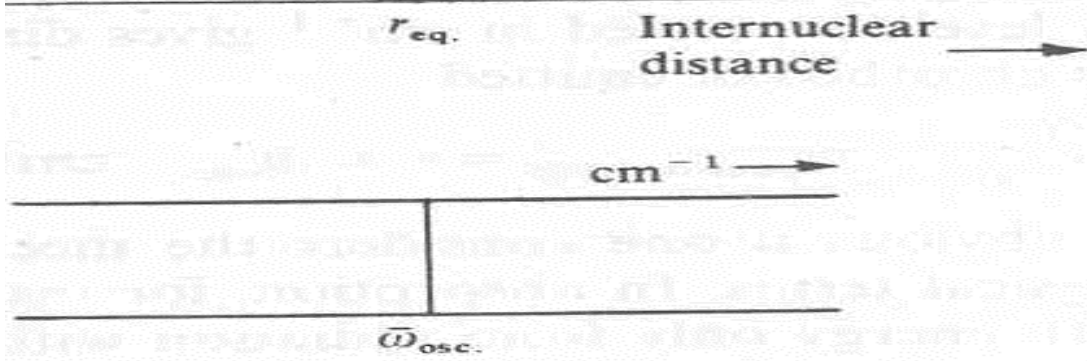
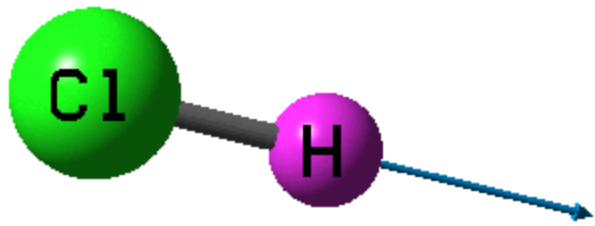
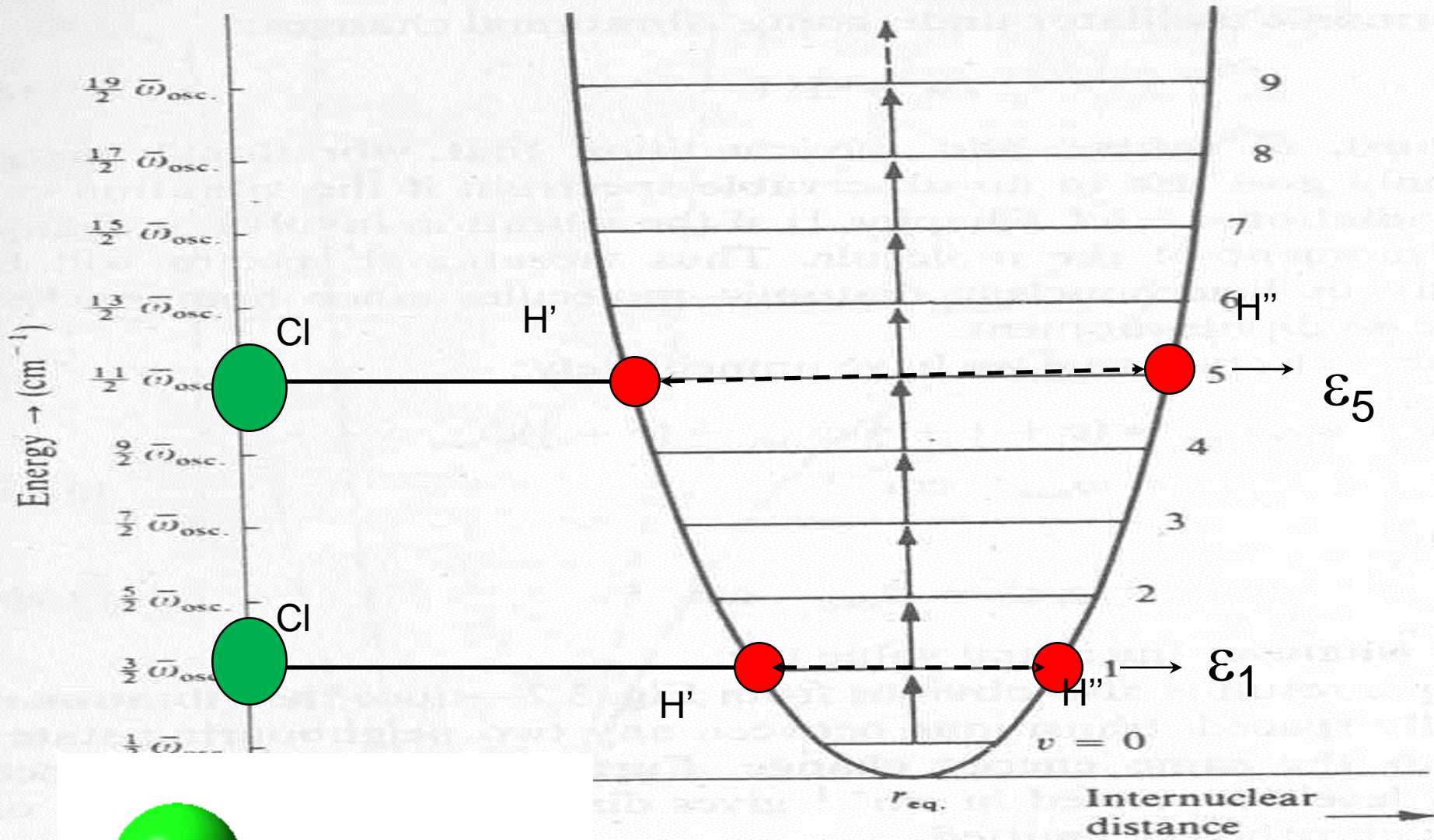
# SHM and Uniform Circular Motion

Springs and Waves behave very similar to objects that move in circles.

The radius of the circle is symbolic of the displacement,  $x$ , of a spring or the amplitude,  $A$ , of a wave.

$$x_{spring} = A_{wave} = r_{circle}$$

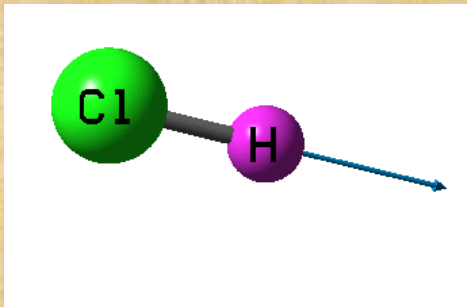






# Vibration of Diatomic Molecule

- Consider a diatomic molecule where two atoms are bounded by bond.
- TWO ATOMS OR PARTICLES BE ALLOWED TO MOVE ONLY ALONG LINE OF THE SYSTEM.
- Let  $x_1$  and  $x_2$  represent displacement of the particles of mass  $m_1$  and  $m_2$  from initial position in which the particles were separated by their equilibrium distance, if Hook's law is assumed for the spring the kinetic and potential energy



$$T = \frac{1}{2} (m_1 \dot{x}_1^2 + m_2 \dot{x}_2^2)$$

$$U = \frac{1}{2} k (x_2 - x_1)^2$$



# Vibration of Diatomic Molecule

• Compression and extension of a bond may be likened to the behaviour of a spring. Assuming that the bond, like the spring, obeys Hooke's law. We may then write

$f = -k (r - r_{eq.})$ . Here  $f$  is a restoring force and  $r$  the inter nuclear distance. In this case the energy curve is parabolic and has the form

$$U = \frac{1}{2} k (r - r_{eq.})^2$$

- This is identical in form to that for single vibrating particle.
- This model of vibrating diatomic molecule-so called simple harmonic oscillator model- while only an approximation, forms an excellent starting point for the discussion of vibrational spectra.

- The zero of the parabolic curve is at  $r=r_e$  and energy in excess of this arises because of extension or compression of the bond.
- During vibration heavy atom stays still and lighter atom generally moves. But only distance between two atoms is important in vibration.
- During extension or compression vibrational frequency will not change because intrinsic vibrational frequency dependent on mass of the system and force constant and independent of amount of distortion.
- All these behaviour are same as the simple harmonic oscillator.

Schrodinger's equation for the harmonic oscillator is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} \left( E - \frac{1}{2} kx^2 \right) \psi = 0$$

$$\text{if } y = \left( \frac{1}{\hbar} \sqrt{km} \right)^{1/2} x \quad x = \sqrt{\frac{2\pi m \nu}{\hbar}} x$$

$$\text{and } \alpha = \frac{2E}{\hbar} \sqrt{\frac{m}{k}} = \frac{2E}{\hbar \nu}$$

$$\Rightarrow \frac{d^2\psi}{dx^2} + (\alpha - y^2) \psi = 0$$

.....(1)

The solution to this equation that are acceptable here are limited by

$$\int_{-\infty}^{\infty} |\psi|^2 dy = 1$$

The mathematical property of (1) is such that a condition must fulfil

$$\alpha = 2v+1 \quad v = 0, 1, 2, 3, \dots$$

The energy level of a harmonic oscillator is given by

$$E_v = \frac{h}{2\pi} \sqrt{\frac{k}{\mu}} \left( v + \frac{1}{2} \right) = h\omega_{osc} \left( v + \frac{1}{2} \right)$$

$$E_v = \left( v + \frac{1}{2} \right) h\omega$$



Schrodinger's equation for the harmonic oscillator is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} \left( E - \frac{1}{2} kx^2 \right) \psi = 0$$

$E_v = (v + \frac{1}{2}) h \omega_{osc}$  joules ( $v = 0, 1, 2, \dots$ ),  
where  $v$  is the vibrational quantum number.

In spectroscopic units

$$\epsilon_v = \frac{E_v}{hc} = \left( v + \frac{1}{2} \right) \bar{\omega}_{osc} \text{ cm}^{-1}$$

# The simple Harmonic Oscillator

In spectroscopic units

$$\epsilon_v = (v + 1/2) \omega_{osc} \text{ cm}^{-1} \dots\dots\dots(3)$$

The lowest energy obtained by putting  $v = 0$  is

$$\epsilon_0 = 1/2 \omega_{osc} \text{ cm}^{-1}$$

Implication from this result is that diatomic molecule( indeed any molecule) can never have zero vibrational energy; the atoms can never be completely at rest relative to each other.

The quantity  $1/2 \omega_{osc} \text{ cm}^{-1}$  is known as the zero point energy.

**Selection Rule:**  $\Delta v = \pm 1$

Vibrational energy changes will only give rise to an observable spectrum if the vibration can interact with radiation.

# The simple Harmonic Oscillator

Applying the selection rule we have immediately:

$$\varepsilon_{v+1 \rightarrow v} = (v+1 + 1/2) \varpi_{\text{osc}} - (v + 1/2) \varpi_{\text{osc}} = \varpi_{\text{osc}} \text{ cm}^{-1}$$

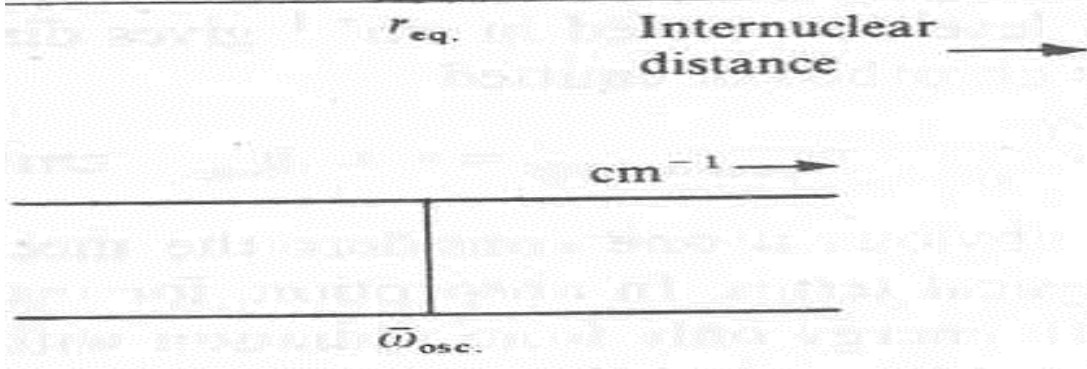
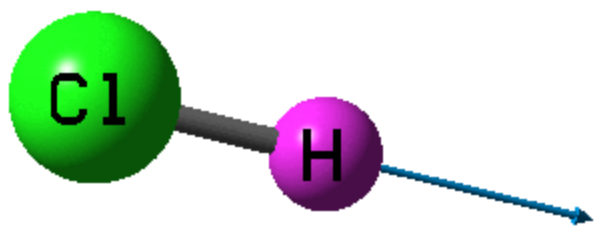
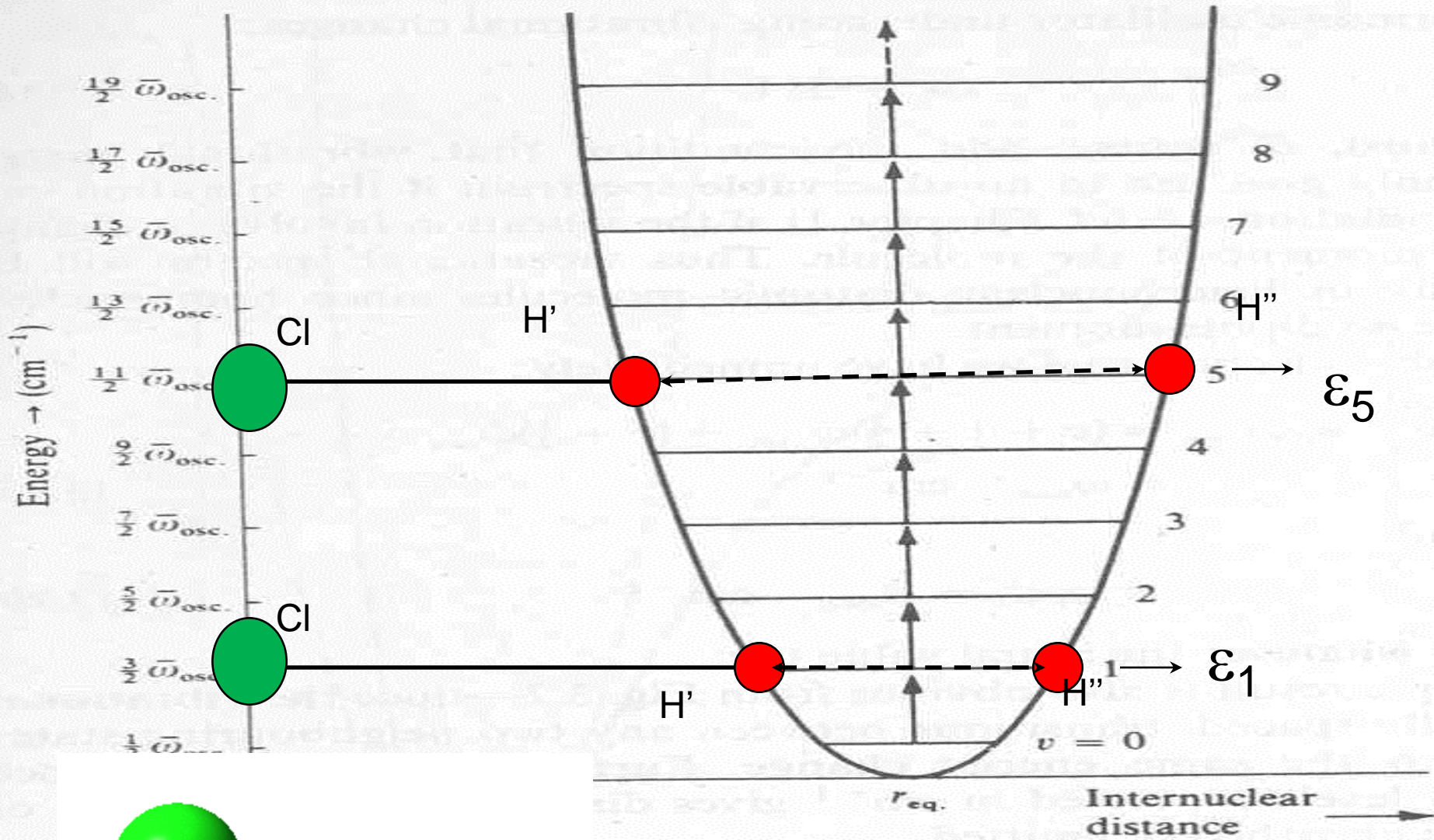
for emission and

$\varepsilon_{v \rightarrow v+1} = \varpi_{\text{osc}} \text{ cm}^{-1}$  for absorption, whatever the initial value of  $v$ .

- Such a simple result is obvious as vibrational levels are equally spaced, Transitions between any two neighbouring states will give rise to same energy change.

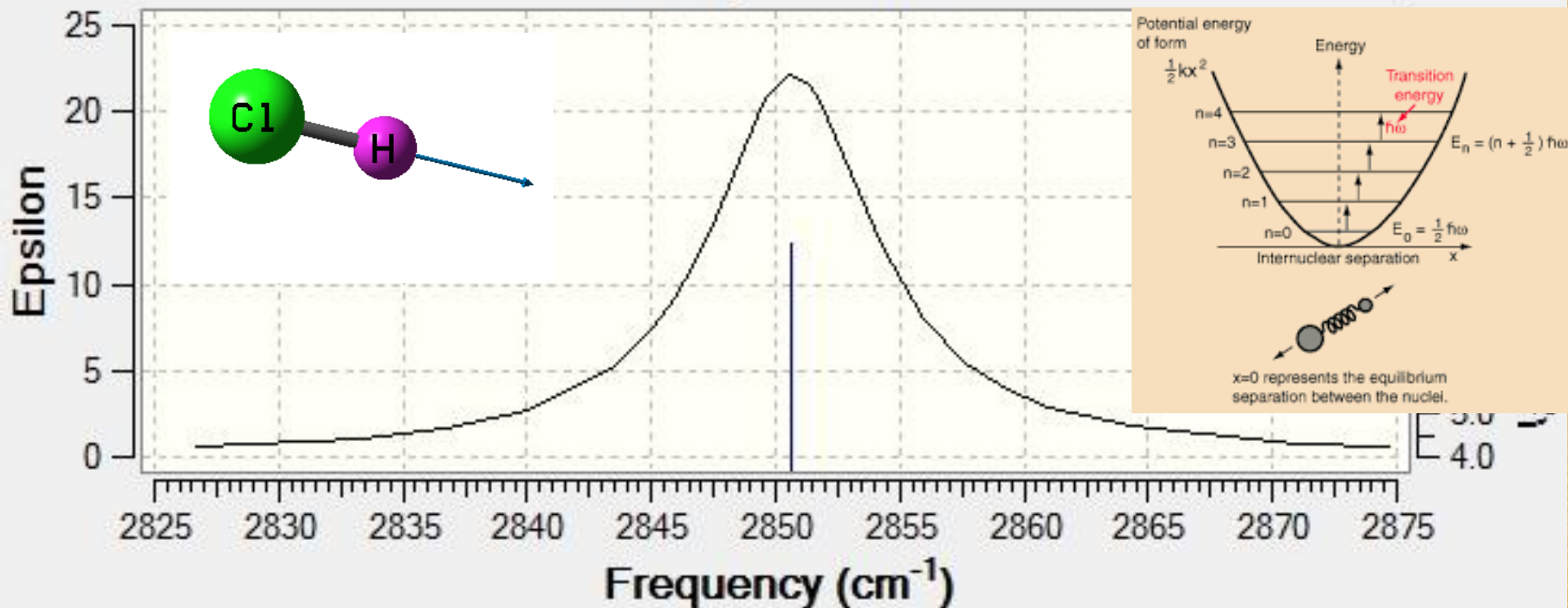
- $\bar{\nu}_{\text{spectroscopic}} = \varepsilon = \varpi_{\text{osc}} \text{ cm}^{-1}$  The vibrating molecule will absorb energy only from radiation with which it can coherently interact and this must be radiation of its own oscillation frequency.





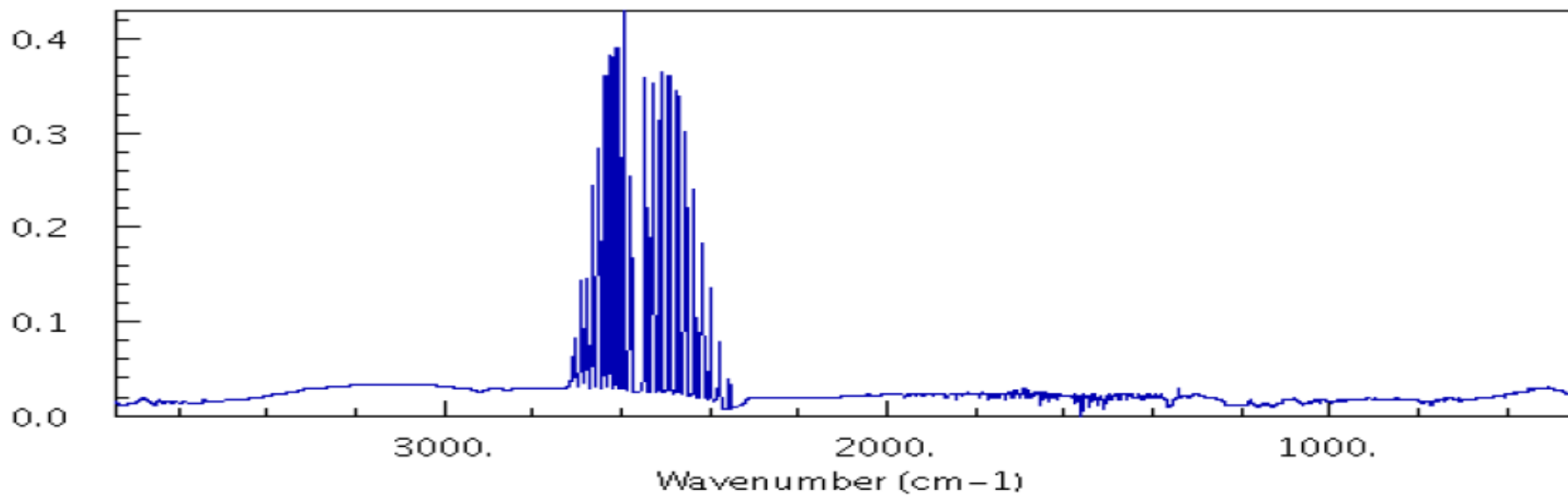


# IR Spectrum



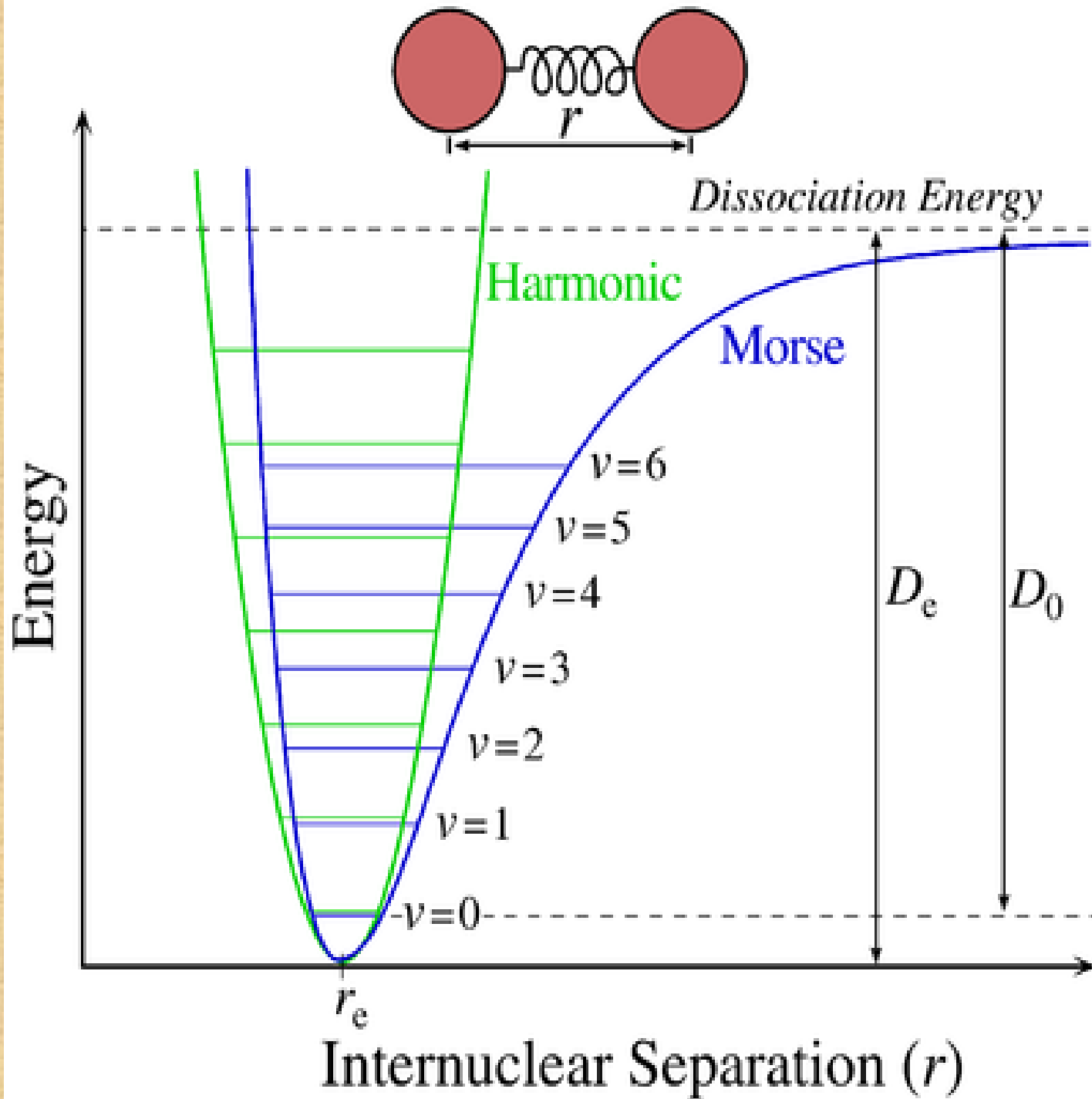
Absorbance

INFRARED SPECTRUM



# The Anharmonic Oscillator

- Real HCl do not obey the laws of simple harmonic motion. If the bonds between the atom is stretched , there comes a point at which it will break- the molecule dissociates into atoms.
- The purely empirical expression which fits the anharmonic curve to a approximation was derived by P.M. Morse, and is called the Morse function:
- $V(r) = D_{eq} \cdot [1 - \exp \{ a ( r_{eq} - r ) \}]^2$ , where  $a$  is a constant for a particular molecule and  $D_{eq}$  is the dissociation energy.



Using Schrodinger equation and potential for anharmonic oscillator, we find the allowed energy levels

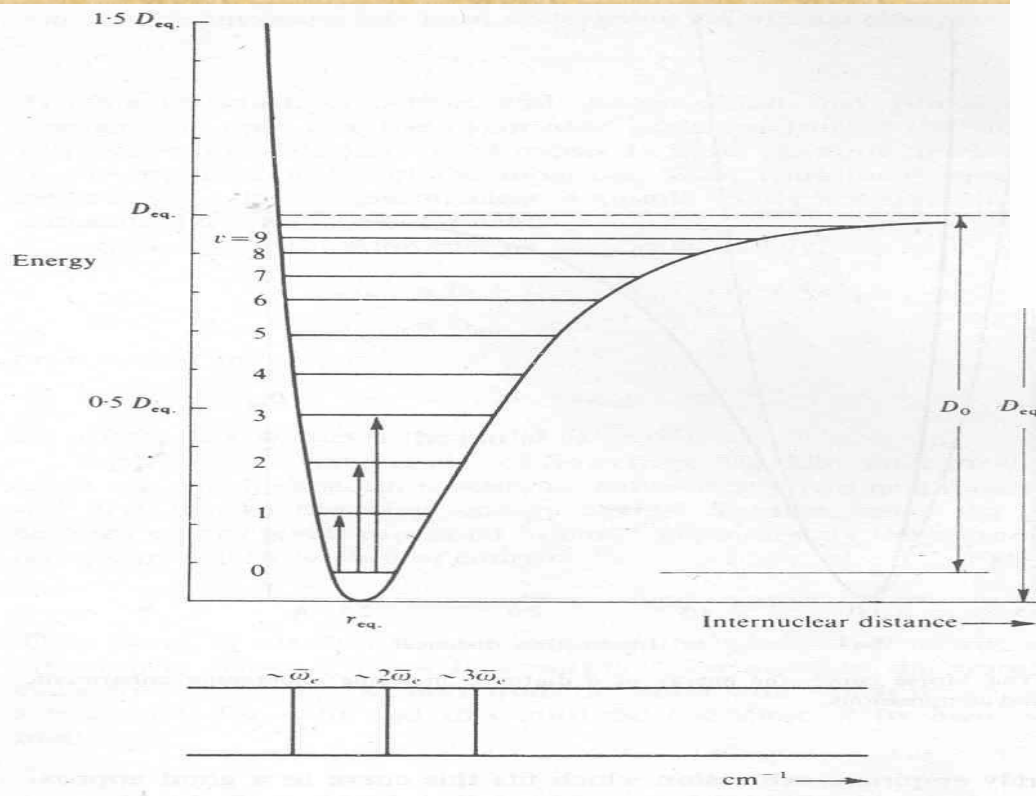
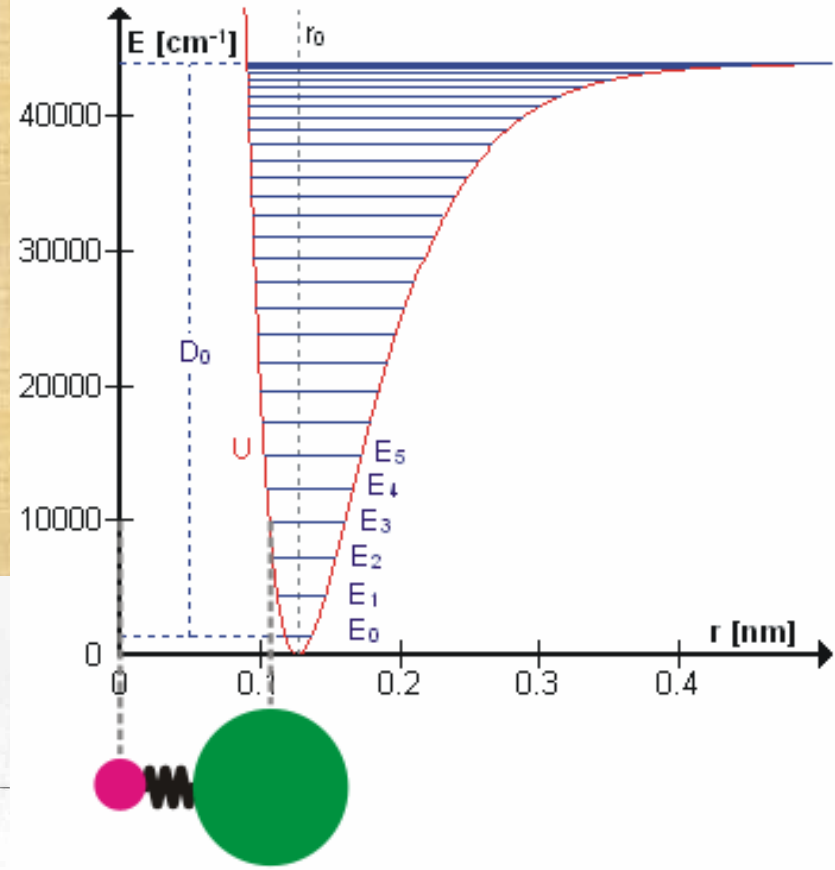
$$\begin{aligned}\varepsilon_v &= \frac{E_v}{hc} \\ &= \left(v + \frac{1}{2}\right) \bar{\omega}_e - \left(v + \frac{1}{2}\right)^2 x_e \bar{\omega}_e + \left(v + \frac{1}{2}\right)^3 y_e \bar{\omega}_e \text{ cm}^{-1}\end{aligned}$$

$x_e$  and  $y_e$  is the corresponding anharmonicity constants which for bond stretching vibrations is always small and positive. More precise expression for the energy levels require cubic, quadratic etc. terms in  $(v + \frac{1}{2})$  with anharmonicity constants  $y_e, z_e$ , etc. rapidly diminishing in magnitude.

$$\bar{\omega}_e = \frac{\omega_{osc}}{c}$$

**Selection Rules:**  $\Delta v = \pm 1, \pm 2, \pm 3, \dots$





1.  $v=0 \rightarrow v=1$ ,  $\Delta v = + 1$  with considerable intensity.

$$\begin{aligned} \Delta \varepsilon &= \varepsilon_{v=1} - \varepsilon_{v=0} \\ &= (1 + \frac{1}{2}) \varpi_e - (1 + \frac{1}{2})^2 \varpi_e x_e - \{ \frac{1}{2} \varpi_e - (\frac{1}{2})^2 \varpi_e x_e \} \\ &= \varpi_e (1 - 2 x_e) \text{cm}^{-1} \dots\dots\dots(a) \end{aligned}$$

2.  $v=0 \rightarrow v=2$ ,  $\Delta v = + 2$  with small intensity.

$$\begin{aligned} \Delta \varepsilon &= \varepsilon_{v=2} - \varepsilon_{v=1} \\ &= (2 + \frac{1}{2}) \varpi_e - (2 + \frac{1}{2})^2 \varpi_e x_e - \{ \frac{1}{2} \varpi_e - (\frac{1}{2})^2 \varpi_e x_e \} \\ &= 2\varpi_e (1 - 3 x_e) \text{cm}^{-1} \end{aligned}$$

3.  $v=0 \rightarrow v=3$ ,  $\Delta v = + 3$  with considerable intensity.

$$\begin{aligned} \Delta e &= \epsilon_{v=3} - \epsilon_{v=0} \\ &= (3 + \frac{1}{2}) \omega_e - (3 + \frac{1}{2})^2 \omega_e x_e - \{ \frac{1}{2} \omega_e - (\frac{1}{2})^2 \omega_e x_e \} \\ &= 3 \omega_e (1 - 4 x_e) \text{cm}^{-1} \dots\dots\dots(c) \end{aligned}$$

To a good approximation since  $x_e \approx 0.01$ , the three spectral lines lie very close to  $\omega_e, 2 \omega_e$  and  $3 \omega_e$ . They are known as fundamental absorption, first overtone and second overtone respectively.

Example: For HCl molecules we have three peaks at  
 at  $2886 \text{ cm}^{-1}$ , at  $5668 \text{ cm}^{-1}$ , and at  $8347 \text{ cm}^{-1}$

# The Vibrations of Polyatomic Molecules.

The spectrum of polyatomic molecules is quite complex.

- **Fundamental Vibrations and their Symmetry:**
- For a molecule containing  $N$  atoms,  $3N$  coordinate values are required to define it completely. If  $3N$  coordinates are fixed then the bond distances and bond angles of the molecule are also fixed then Molecule is said possessing  $3N$  degree of freedom.
- ***Degrees of freedom*** is a general term used in explaining dependence on specific parameters and implying the possibility of counting the number of those parameters.

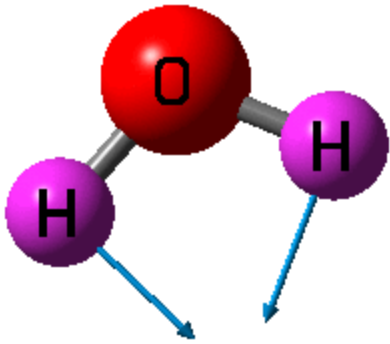


- If the molecule is free to move in three dimensional space without change of shape such that the molecule has only translational change. so the degrees of freedom will be  $3N-3$ .
- As there are 3 translations and rotations which do not form internal vibrations so we have
- For Non-linear:  $3N - 6$  fundamental vibrations.
- For Linear :  $3N - 5$  fundamental vibratons as rotation about the bond axis is restricted.

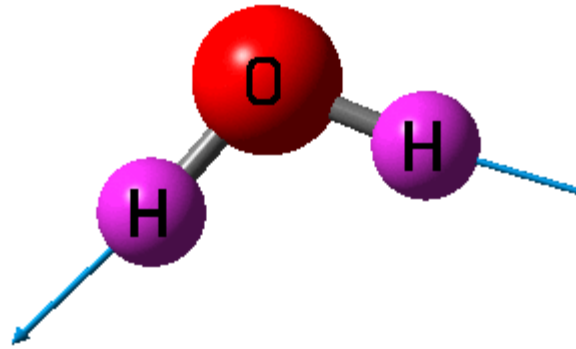
Since an N atomic molecule has N-1 bonds between its atoms, N-1 of the vibrations are bond stretching, the other  $2N-5$ (nonlinear) or  $2N-4$ (linear) are bending motions.

Examples: For diatomic molecule,  $N=2$ ,  $3 \times 2 - 5 = 1$ , only one fundamental vibration.

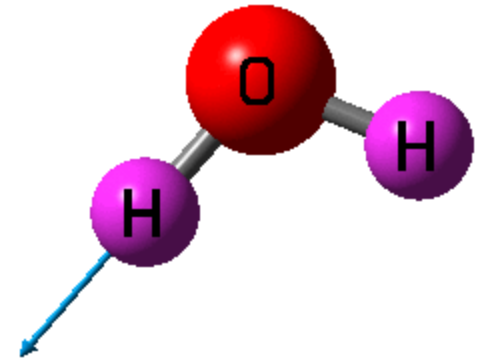
- For water,  $N=3$ ,  $3 \times 3 - 6 = 3$  allowed fundamental vibrational modes.
- These vibrational modes are also referred to as the normal modes of vibration of the molecule.
- By utilizing the symmetry elements in the molecules each motion may be leveled symmetric or antisymmetric.



Bending  
 $\delta$



Symmetric stretching  
 $\nu_{S(OH)}$



Asymmetric stretching  
 $\nu_{AS(OH)}$

# IR active modes

frequency ( $\text{cm}^{-1}$ )

Intensity

Mode

1800.00

265.83

$\delta$

3810.00

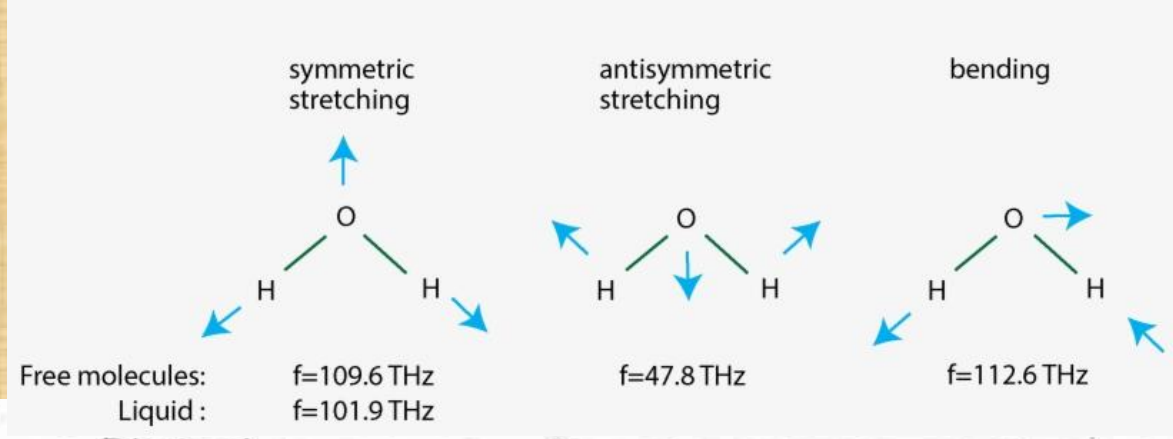
10.00

$\nu_{S(OH)}$

3945.00

70.84

$\nu_{AS(OH)}$



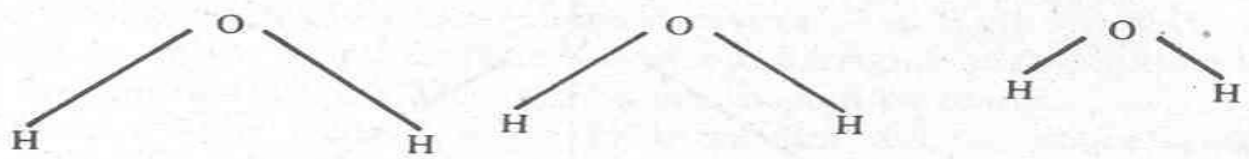
Vibrational Mode

Distorted Molecule

Normal Molecule

Distorted Molecule

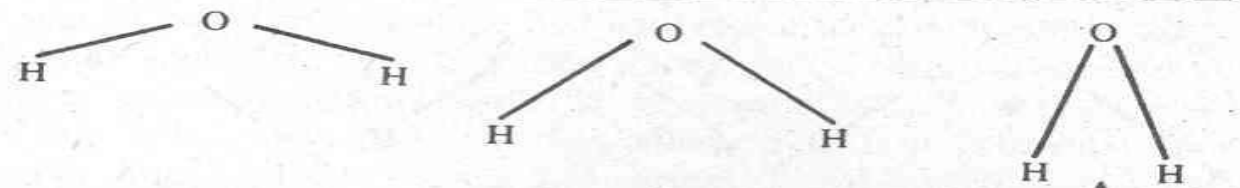
$\nu_1$



Dipole



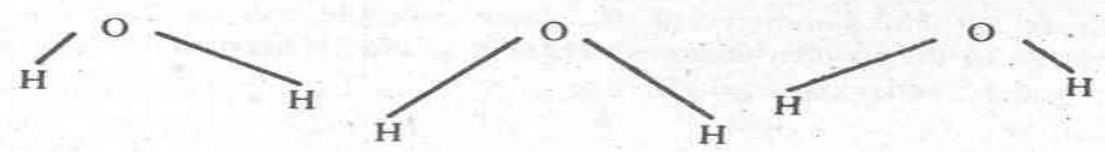
$\nu_2$



Dipole



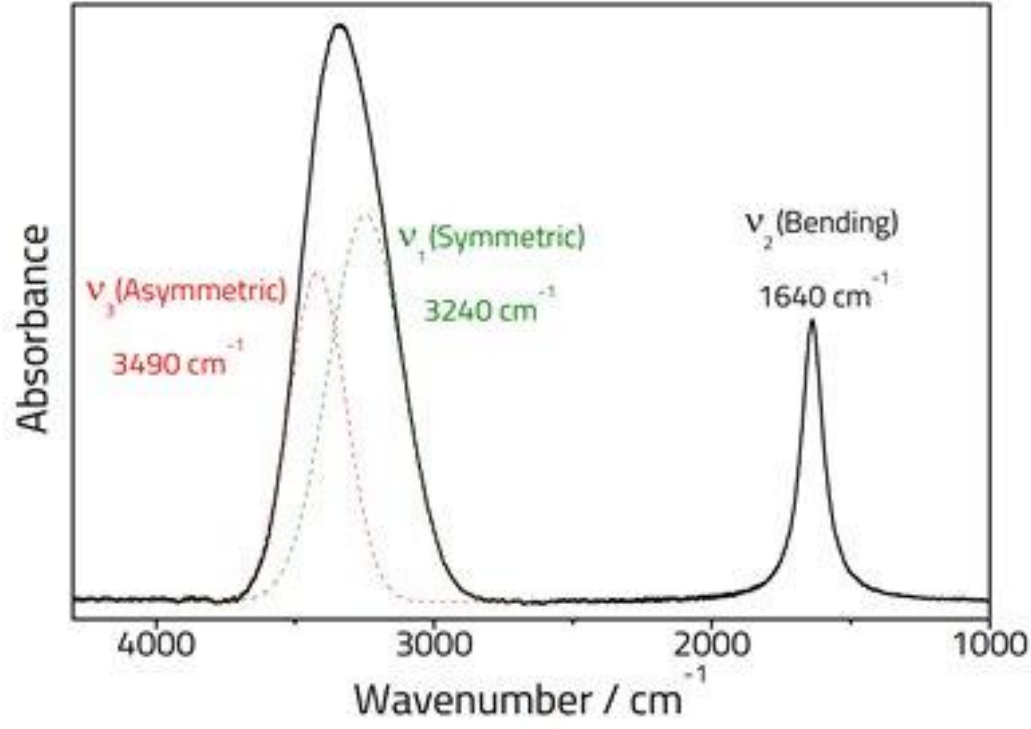
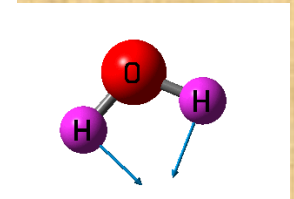
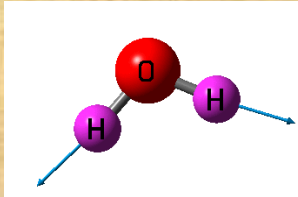
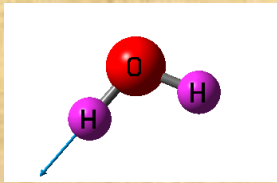
$\nu_3$



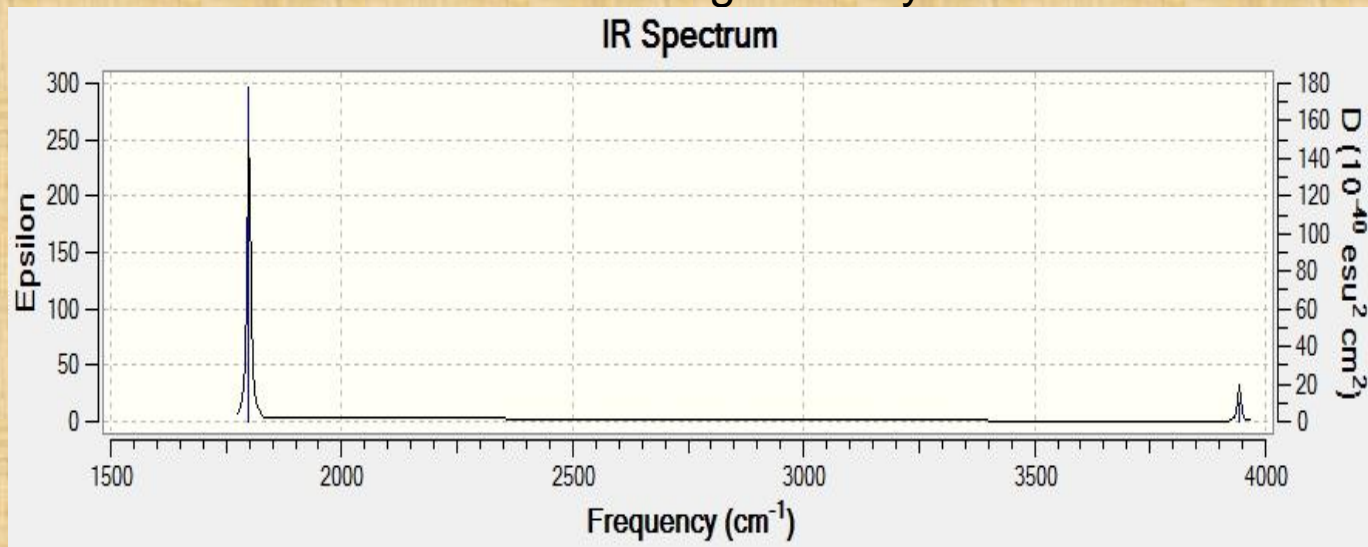
Dipole



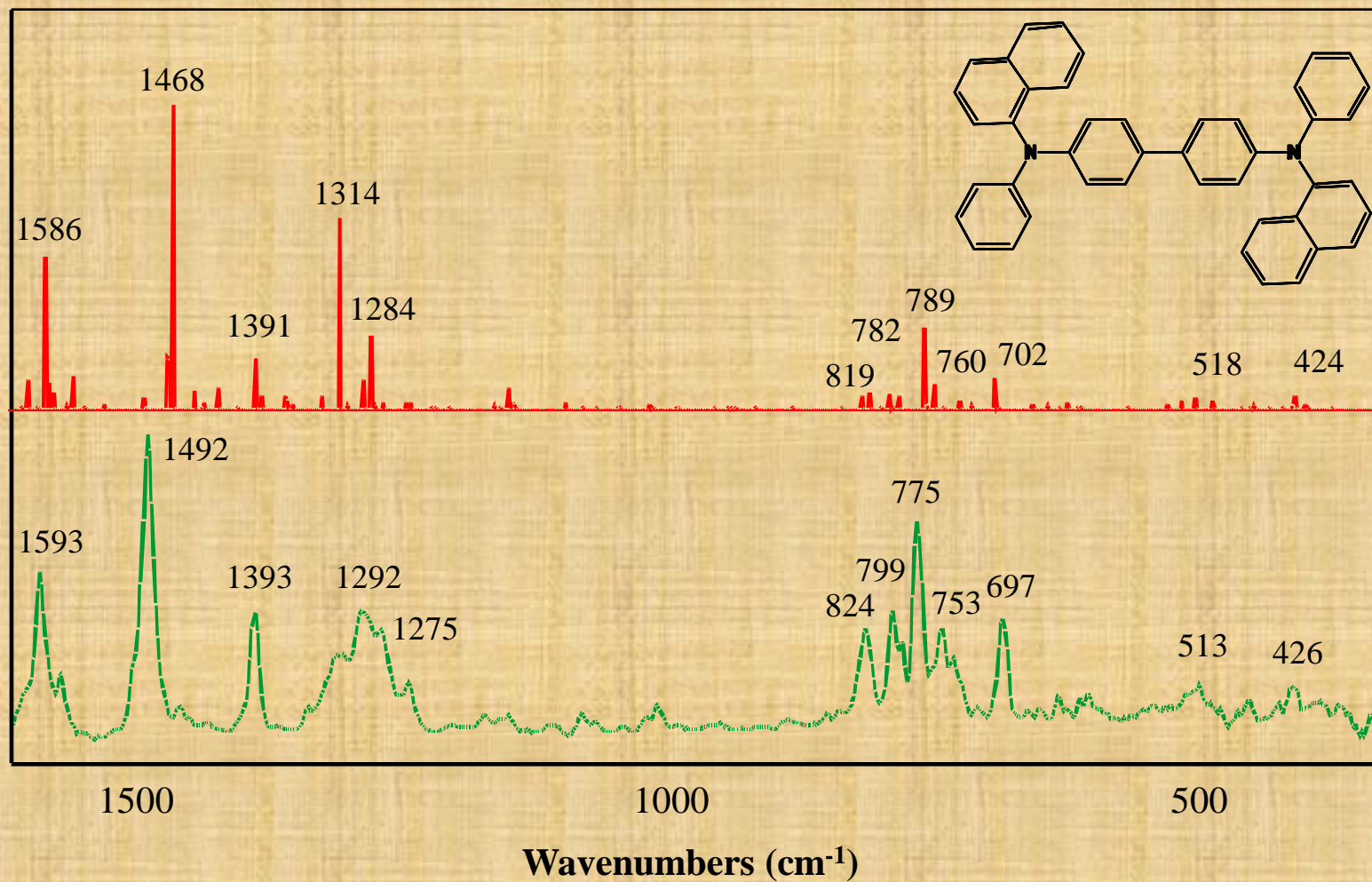




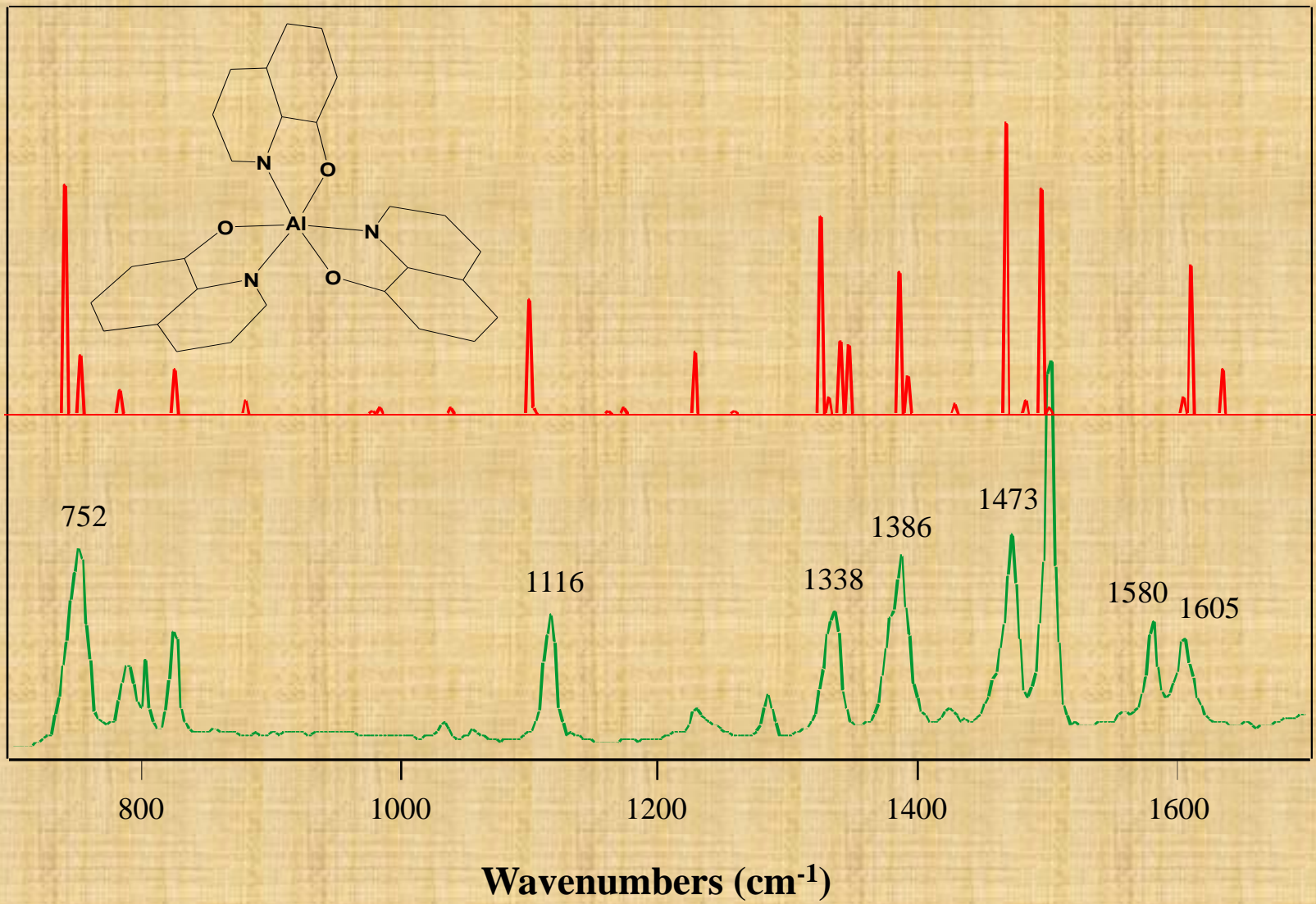
The spectrum of liquid water recorded with a 2 m m thick normal liquid cell with ZnSe windows in transmission mode (red spectrum) and original ATR spectrum (blue spectrum) both normalized to the OH stretching intensity.



# Reflection-Absorption Infrared Spectrum of NPB



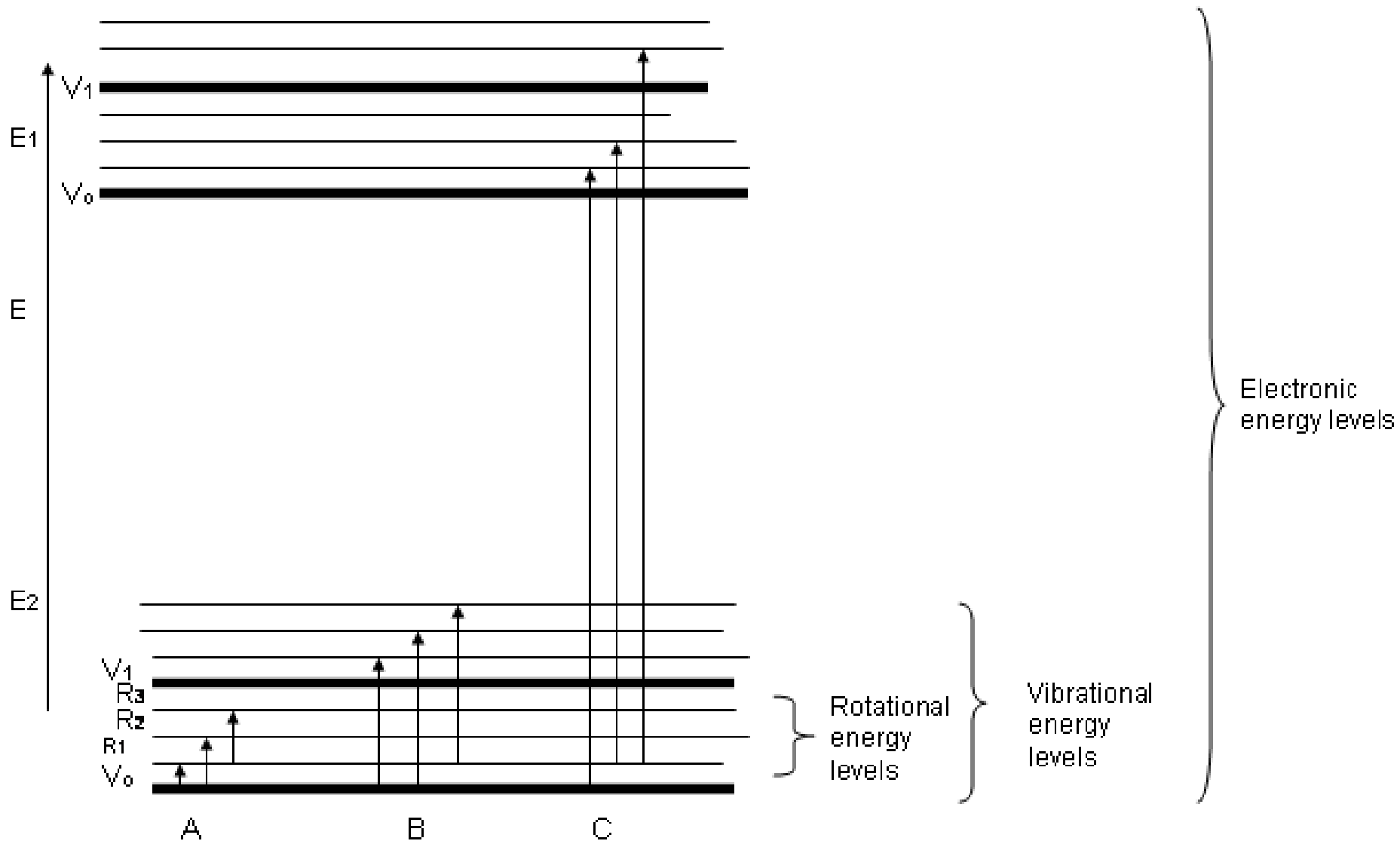
# Reflection-Absorption Infrared Spectrum of AIQ3



# The diatomic vibrating Rotator

- In liquid molecules are very close together, so interaction during rotation produce the change in bond length and so the vibrational spectra.
- Energy needed for rotational spectra is so small that at room temperature the molecule get sufficient amount of energy to rotate.
- In gas phase the distance between the molecules is quite large so to see vibrational spectra excitation energy is needed.





# The diatomic vibrating Rotator

**Born-Oppenheimer approximation:** A diatomic molecule can execute rotations and vibrations quite independently. The combined rotational vibrational energy is simply the sum of the separate energies:

$$E_{\text{total}} = E_{\text{rot.}} + E_{\text{vib.}} \quad (\text{joules})$$

$$\varepsilon_{\text{total}} = \varepsilon_{\text{rot.}} + \varepsilon_{\text{vib.}} \quad (\text{cm}^{-1})$$

Taking the separate expression for  $\varepsilon_{\text{rot.}}$  and  $\varepsilon_{\text{vib.}}$  From previous discussions, we have

$$\begin{aligned} \varepsilon_{J,v} &= \varepsilon_J + \varepsilon_v \\ &= BJ(J+1) - DJ^2(J+1)^2 + \dots + (v + \frac{1}{2}) \omega_e - \\ &\quad (v + \frac{1}{2})^2 \omega_e x_e \text{ cm}^{-1} \end{aligned}$$

- If we ignore the effect of centrifugal distortion and anharmonicity then the energy levels of a diatomic molecule is

$$E_{v,J} = \left( v + \frac{1}{2} \right) \eta \sqrt{\frac{k}{\mu}} + J(J + 1) \frac{\eta^2}{2I}$$

**Selection Rule:** The selection rules for the combined motions are the same as those for each separately

$$\Delta v = \pm 1 \quad \Delta J = \pm 1,$$

The  $v=0$  to  $v=1$  transition fall into two categories, the P branch in which  $\Delta J = -1$  (that is  $J$  TO  $J-1$ ) and the R branch In which  $\Delta J = +1$  ( $J$  TO  $J+1$ )

$$\nu_P = \frac{E_{1,J-1} - E_{0,J}}{h} = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}} + [(J-1)J - J(J+1)] \frac{\eta}{4\pi I}$$

$$= \nu_0 - J \frac{\eta}{2\pi I}$$

$$\nu_R = \frac{E_{1,J+1} - E_{0,J}}{h} = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}} + [(J+1)(J+2) - J(J+1)] \frac{\eta}{4\pi I}$$

$$= \nu_0 + (J+1) \frac{\eta}{2\pi I}$$

There will be no line at  $\nu = \nu_0$  because transition for  $\Delta J=0$  are forbidden in diatomic molecules.



# The diatomic vibrating Rotator

An analytical expression for the spectrum may be obtained by applying the selection rules to the energy levels. Considering only the  $v=0 \rightarrow v=1$  transition we have in general

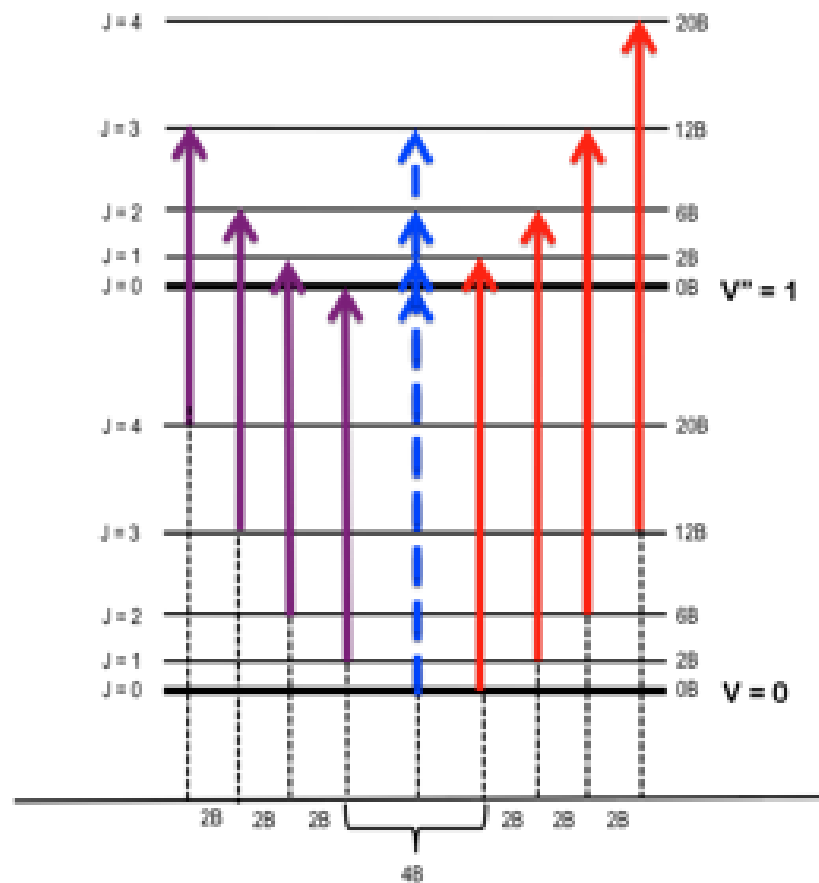
$$\begin{aligned} \varepsilon_{J,v} &= \varepsilon_{J', v=1} - \varepsilon_{J'', v=0} \\ &= B J'(J'+1) - D J'^2(J'+1)^2 + 1 \frac{1}{2} \omega_e - 2 \frac{1}{4} \omega_e x_e \\ &- \{ B J''(J''+1) - D J''^2(J''+1)^2 + \frac{1}{2} \omega_e - \frac{1}{4} \omega_e x_e \} \text{cm}^{-1} \end{aligned}$$

$= \omega_0 + B(J' - J'')(J' + J'' + 1) \text{ cm}^{-1}$  Considering  $D$  negligible.

P branch:  $\Delta J = -1$

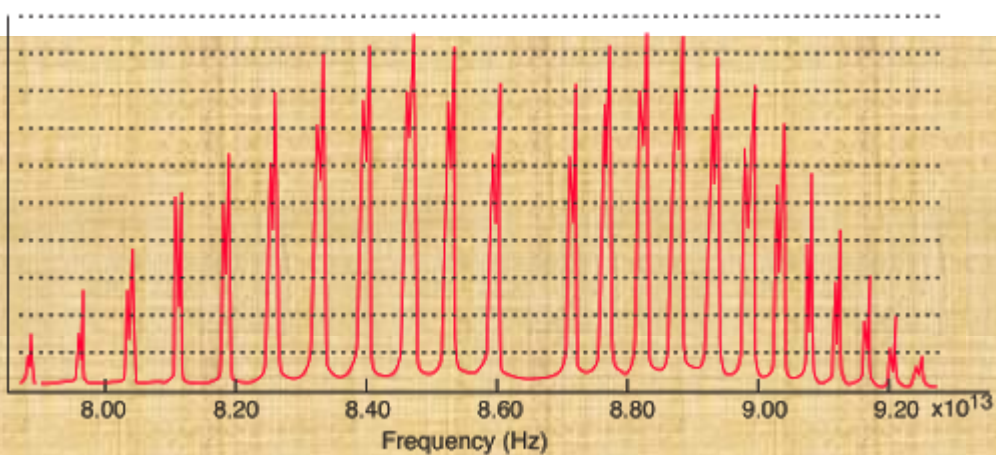
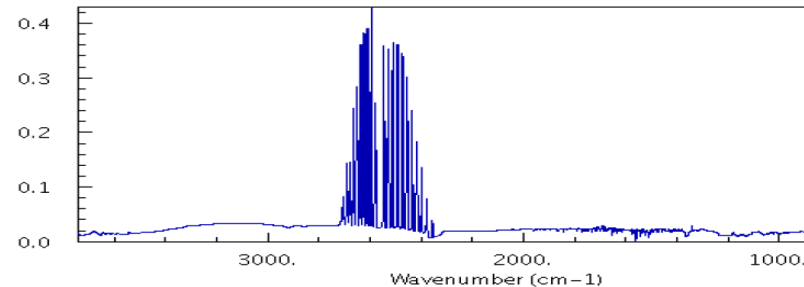
Q branch:  $\Delta J = 0$

R branch:  $\Delta J = +1$



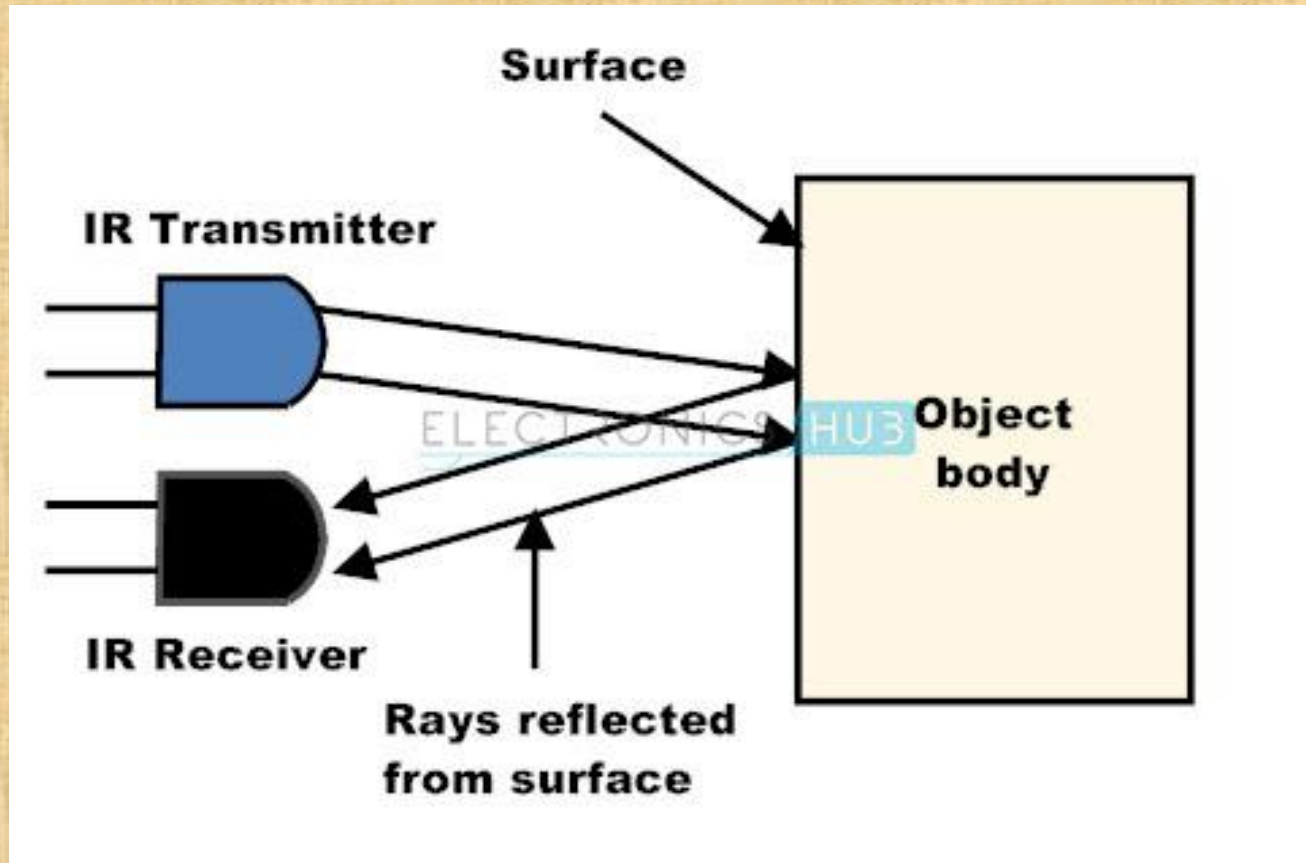
Absorbance

INFRARED SPECTRUM

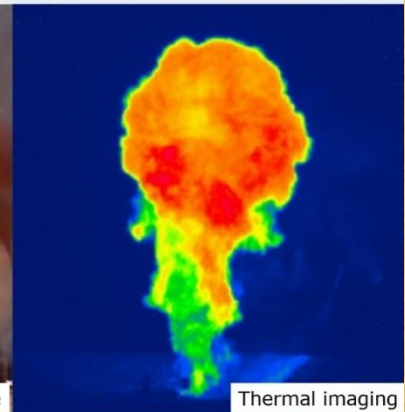
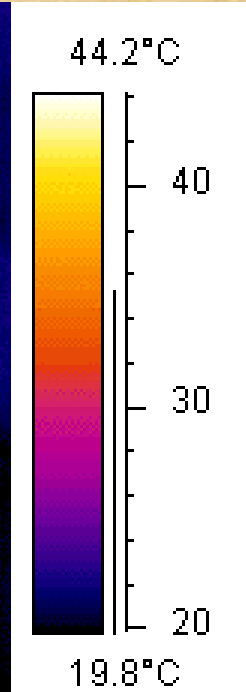
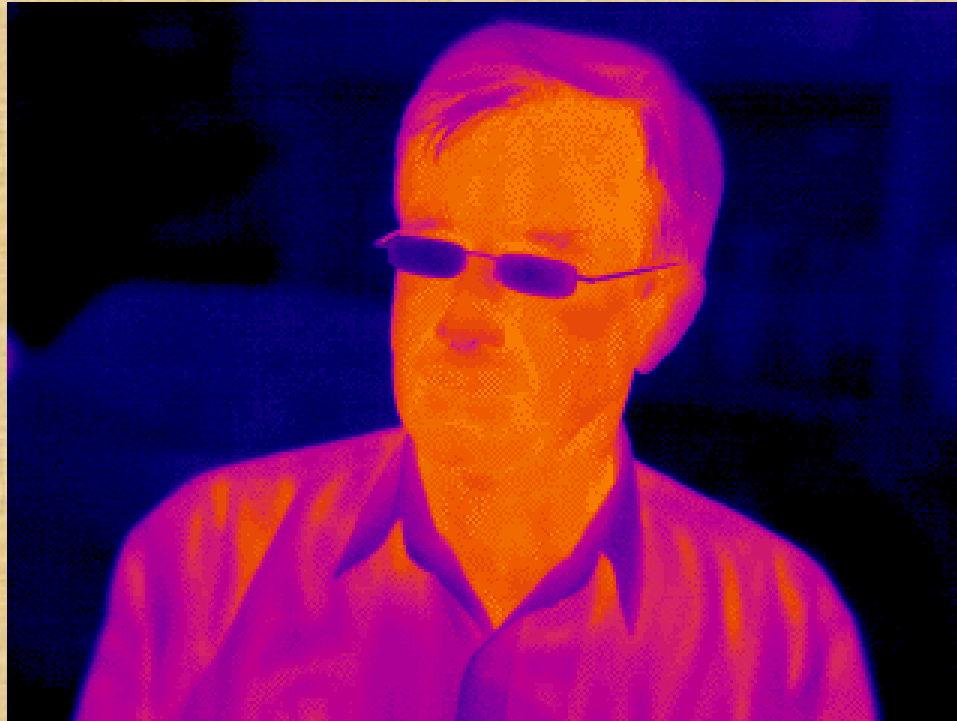


# Applications

## IR Detector



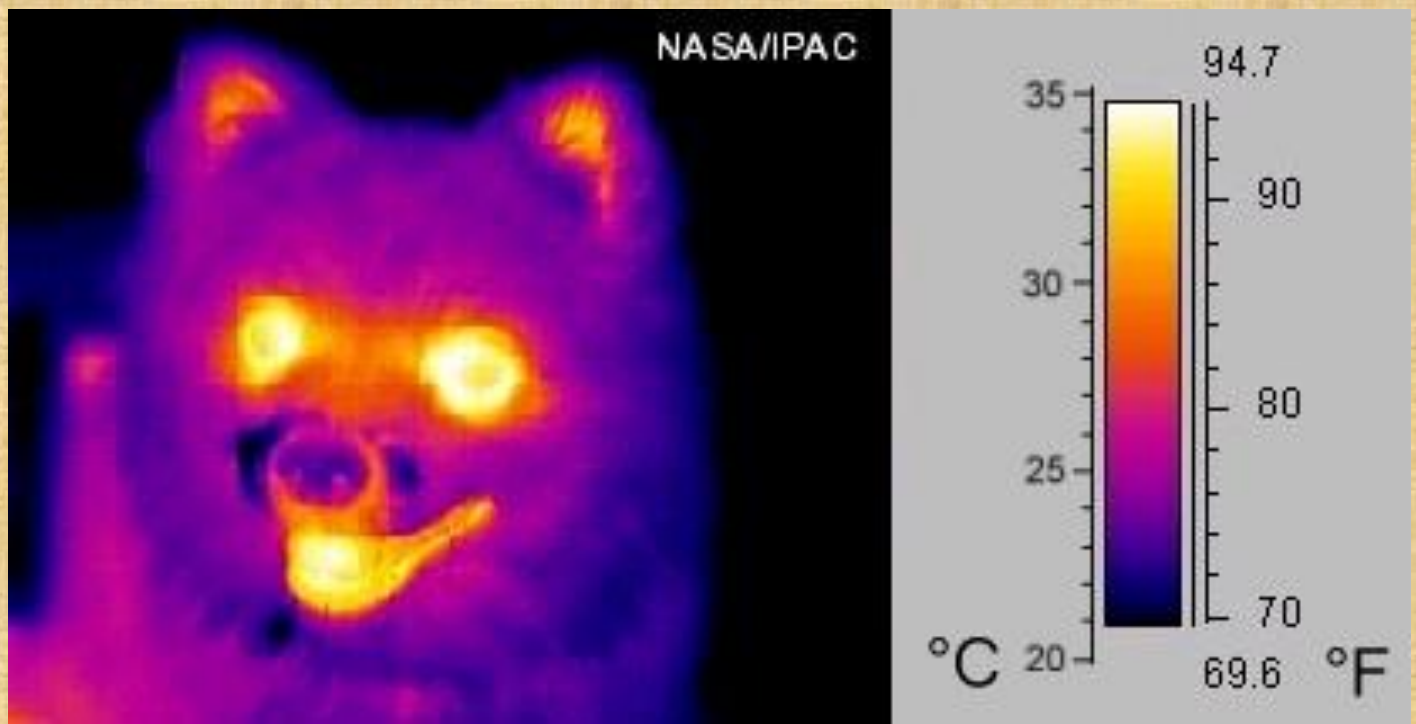
## Body temperature detection by Infrared modes

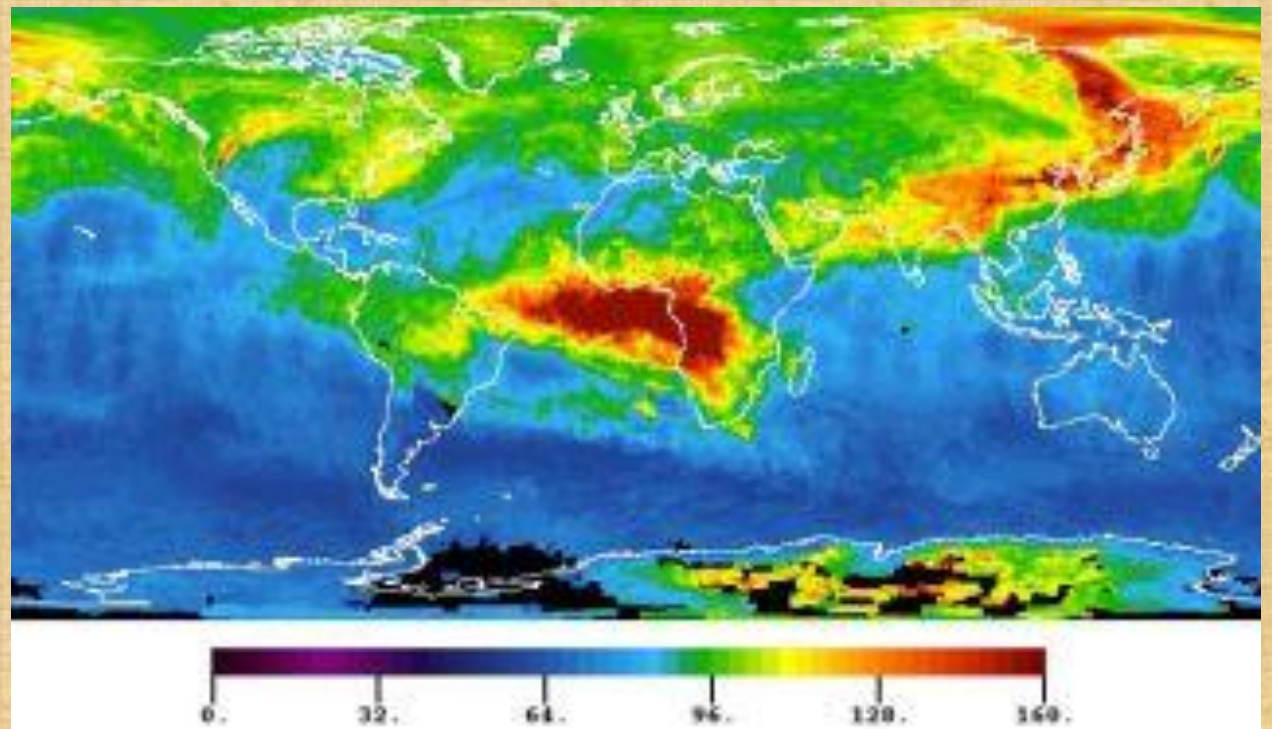


Video frame

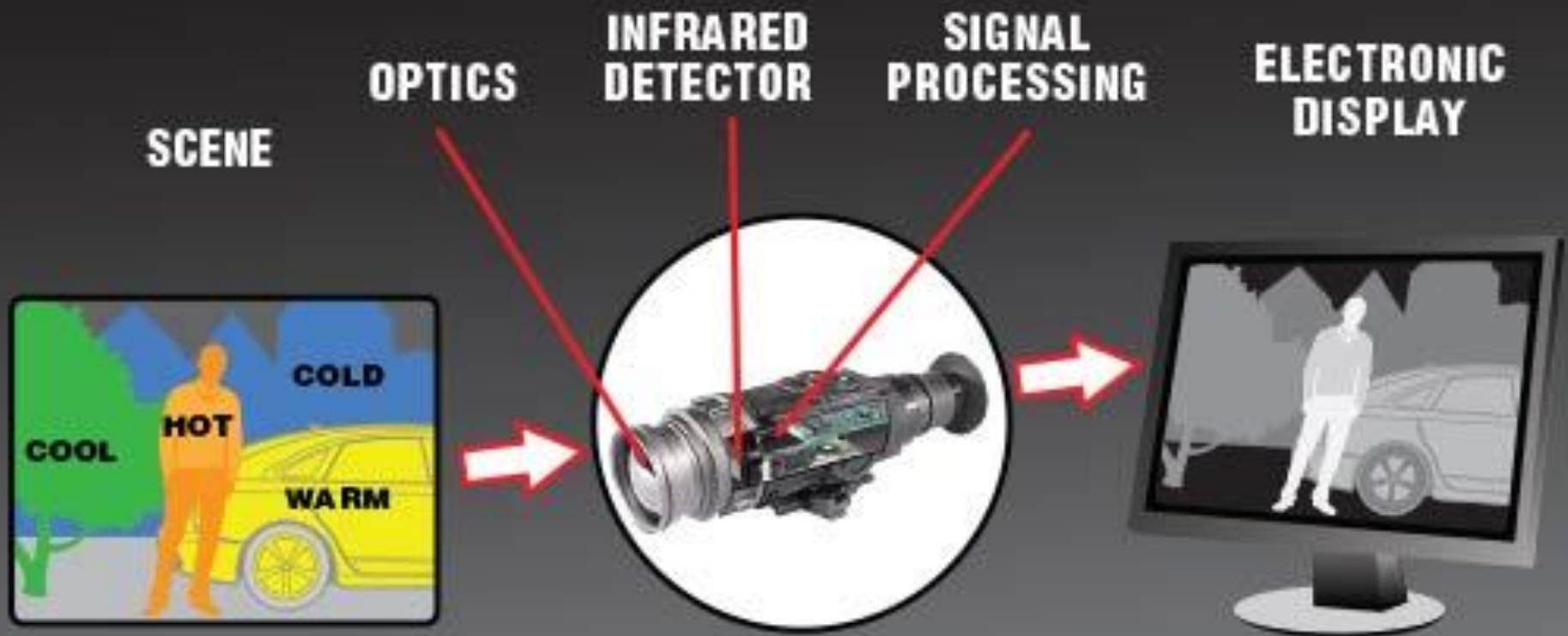
Thermal imaging









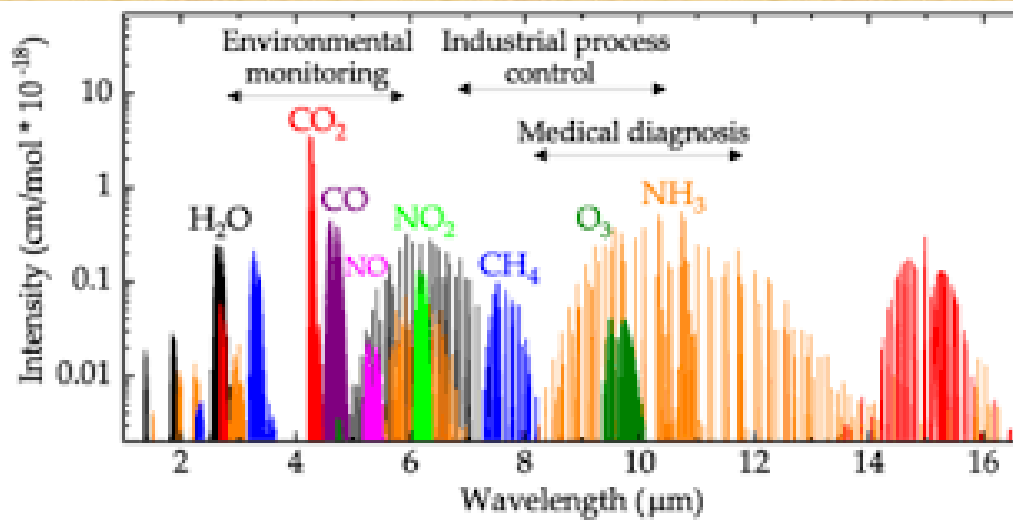


Infrared energy is emitted proportionately to the temperature of an object.

Infrared energy from objects in the scene is focused by an optic lens. The energy is focused onto an infrared detector. The information is passed to sensor electronics for image processing.

The signal processing circuitry translates the infrared detector data into an image that can be viewed on an electronic display.

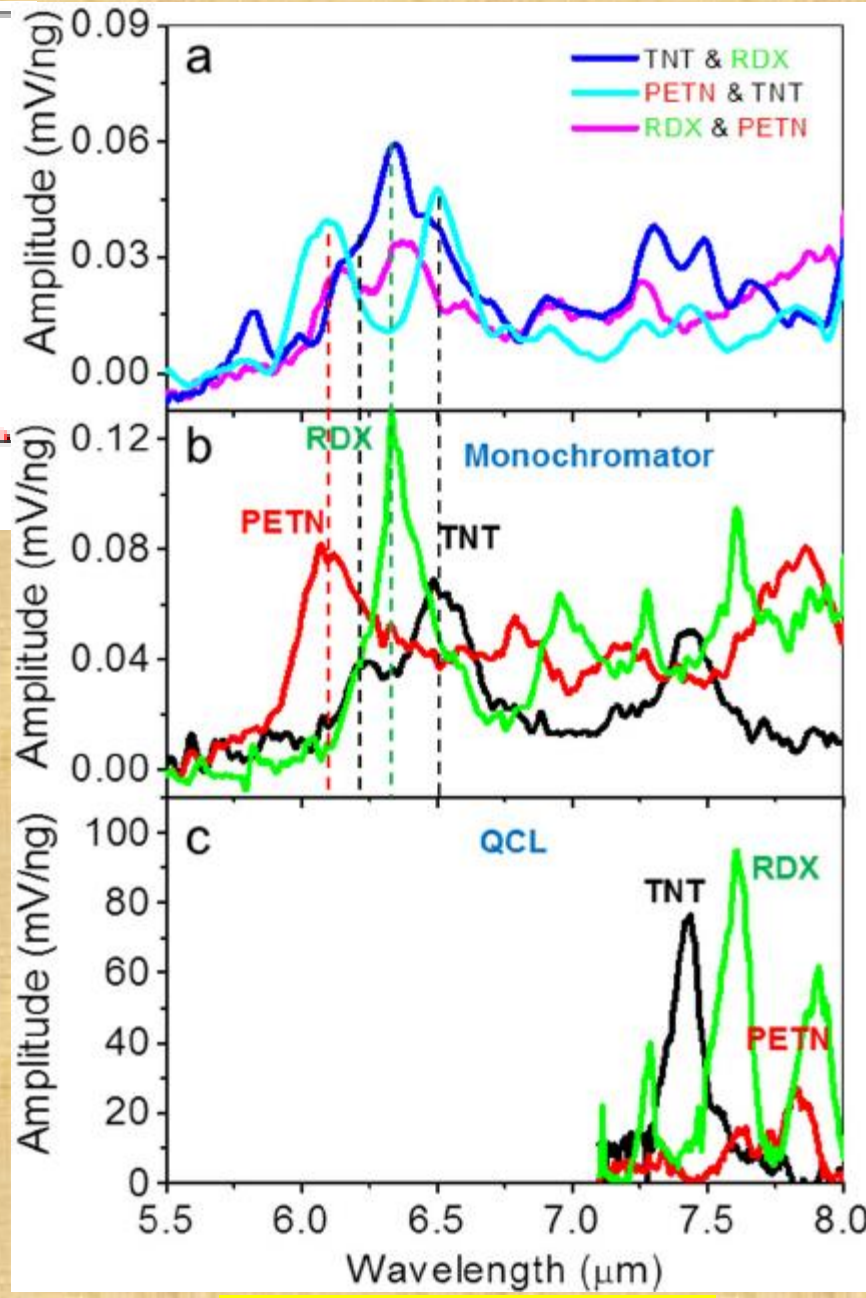
**IR imaging by temperature variation**



**Pollution detection by IR modes**



**Bomb or bomb material detection**



**Chemical detection**

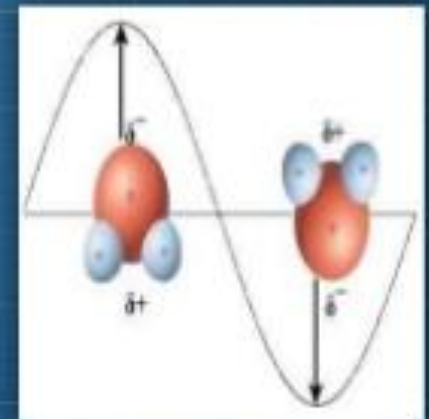
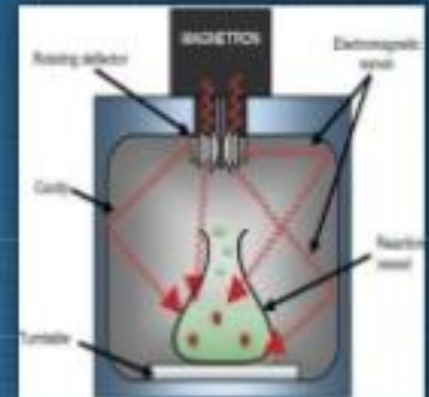


# Microwave Oven

## ► Working Principles

- Microwave oven works by passing non-ionizing microwave radiation, usually at a frequency 2.45 GHz (a wavelength of 12.24 cm), through the food...water, fat & other substances in the food absorb energy from the microwaves in a process called dielectric heating.

- Many molecules (water) are electric dipoles, meaning that they have “+” charge at one end & “-” charge at other end therefore rotate as they try to align themselves & this rotation put them into motion which creates heat.



# Recent Publications

1. M. Rana, A. Jain, V. Rani, **P. Chowdhury**; Glutathione capped core/shell CdSeS/ZnS quantum dots as a medical imaging tool for cancer cells; *Inorganic Chemistry Communications* (2020), 112, 107723 .[Index in scopus, Impact factor: 1.794].
2. M. Rana, **P. Chowdhury**; Studies on Size Dependent Structures and Optical Properties of CdSeS Clusters; *Journal of Cluster Science* (2020), <https://doi.org/10.1007/s10876-019-01719-0>. [Index in scopus, Impact factor: 2.15]
3. Pooja, M, Rana.M, **P. Chowdhury**; Optical and Structural Investigation of CdTe Quantum Dots in Freezed Solid Phase Between PVA Polymer Matrix; *AIP Conference Proceedings*, (2020), (in press) .[Index in scopus, Impact factor: 0.40].
4. M. Rana, **P. Chowdhury**, L-glutathione capped CdSeS/ZnS quantum dot sensor for the detection of environmentally hazardous metal ions; *J of Luminescence*, (2019), Vol 206. 105-112 [Index in scopus, Impact factor: 2.367].
5. Pooja, M, Rana.M, **P. Chowdhury**; Influence of size and shape of optical and electronic properties of CdTe quantum dots in aqueous; *AIP Conference Proceedings*, (2019), 2136, 040006 (2019); <https://doi.org/10.1063/1.5120920>; .[Index in scopus, Impact factor: 0.40].
6. M. Rana, Pooja, **P. Chowdhury**; Investigation on Nonlinear Optical Responses of Different Pyrrole Derivatives: *AIP Conference Proceedings*, (2019), A Computational Study; **2136**, 040005 (2019); <https://doi.org/10.1063/1.5120919>; .[Index in scopus, Impact factor: 0.40].
7. **Rana M.**, Chowdhury P., “*Perturbation of hydrogen bonding in hydrated pyrrole-2-carboxaldehyde complexes*”, Journal of Molecular Modelling, vol. 23, pp. 216-227, 2017. (Thomson Reuters I. F. = 1.425, h-index = 54, h5-index = 34, Published by Springer, Indexed in SCI and SCOPUS).
8. **Rana M.**, Chowdhury P., “*Effects of hydrogen bonding between pyrrole-2-carboxaldehyde and nearest polar and nonpolar environment*”, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, vol. 185, pp. 198–206, 2017. (Thomson Reuters I. F. = 2.536, h-index = 89, h5-index = 53, Published by Elsevier, Indexed in SCI and SCOPUS).
9. **Rana M.**, Singla N., Pathak A., Dhanya R., Narayana C., Chowdhury P., “*Vibrational-electronic properties of intra/inter molecular hydrogen bonded heterocyclic dimer: An experimental and theoretical study of pyrrole-2-carboxaldehyde*”, Vibrational Spectroscopy, vol. 89, pp. 16-25, 2017. (Thomson Reuters I. F. = 1.74, h-index = 62, h5-index = 23, Published by Elsevier, Indexed in SCI and SCOPUS).
10. **Rana M.**, Singla N., Chatterjee A., Shukla A., Chowdhury P. “*Investigation of nonlinear optical (NLO) properties by charge transfer contributions of amine functionalized tetraphenylethylene*” Optical Materials, vol. 62, pp. 80-89, 2016. (Thomson Reuters I. F. = 2.238, h-index = 84, h5-index = 35, Published by Elsevier, Indexed in SCI and SCOPUS).