

Basics of Quantum Chemistry.



Quantum mechanics -

Science of motion of micro particles.

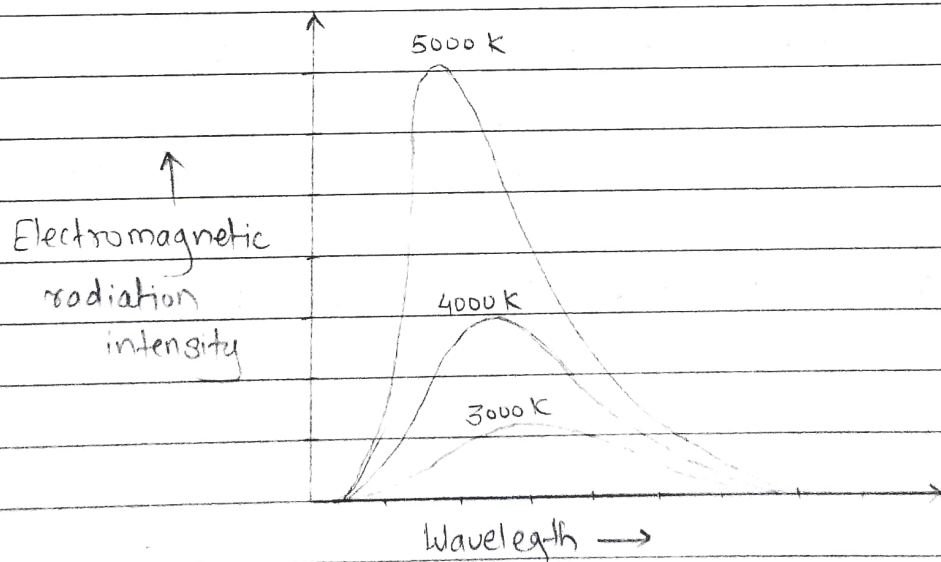
Quantum mechanics can interpret structure, spectral behaviour and even reaction of atoms and molecules in terms of motion of micro particles like electrons and protons.

Blackbody radiation-

Can absorb all the radiation that falls on it.

Intensity of radiation, i.e. total radiation emitted per unit surface area, from a black body depends only on temperature (T) and is independent of the nature of solid.

Distribution of energy in the blackbody radiation-



This distribution is described in terms of function $\rho(\nu) d\nu$ which denotes the density of radiant energy in the frequency range ν and $d\nu + \nu$. i.e. amount of radiation per unit volume of black body chamber at a temperature T .

Lord Rayleigh (1900) first attempted at deriving an equation for distribution of radiation density in terms of classical laws of mechanics.

This derivation based on two theorems -

- i) Theorem of stationary waves in a hollow space
- ii) Theorem of equipartition of energy.

If the walls of black body chamber are assumed to be composed of large no. of harmonic oscillator that emit and absorb radiation continuously.

then the radiation density is given by -

$$p(\nu) d\nu = \bar{E} n(\nu) d\nu$$

↑ average ene. of oscillator

$n(\nu)$ ← no. of possible vibrations per unit volume

We can write, $\bar{E} = k_B T$

$$n(\nu) = \frac{8\pi\nu^2}{c^3}$$

∴ Radiation density can be written as -

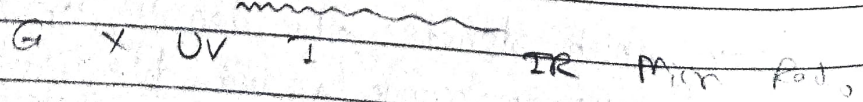
$$p(\nu) d\nu = \frac{8\pi\nu^2}{c^3} \cdot k_B T \cdot d\nu$$

This is Rayleigh-Jeans law of radiation.

Valid at small ν - i.e for large wavelength

not applicable to small wavelength

V I B G Y O R



Planck's law of radiation -

In Oct. 1900, Max Planck proposed a new empirical formula as -

$$P(\nu) d\nu = \frac{a\nu^3}{\exp(b\nu/T) - 1}$$

where a , and b are constants.

He proposed that black body chamber was filled not only with radiation but also with molecules of perfect gas, and dipole oscillators of molecular dimensions constituting the blackbody.

Planck calculated no. of oscillator per unit volume - $\frac{8\pi\nu^2}{c^3}$

So, radiation density as

$$P(\nu) = \frac{8\pi\nu^2}{c^3} \bar{E}(\nu)$$

Planck calculated mean energy \bar{E} of the oscillators. Planck gave up hypothesis of continuous emission of radiation by oscillators and assumed that they emitted ene. only when they acquired certain min. ene. E or integral multiple of it, nE .

He calculated \bar{E} as -

$$\bar{E} = \frac{E}{\exp(E/K_B T) - 1}$$

\therefore Energy density relation becomes.

$$P(\nu) d\nu = \frac{8\pi h \nu^3}{c^3} \cdot \frac{1}{\exp(h\nu/K_B T) - 1} d\nu$$

which gives - $a = \frac{8\pi h}{c^3}$ & $b = \frac{h}{K_B}$

.... Since $E = h\nu$.

Photoelectric effect -

Wave-particle duality of radiation

Photoelectric effect -

When a beam of electromagnetic radiation of a particular frequency falls on a metal surface, electrons are ejected.

i) Photoelectric emission of e^- s is possible only with light of certain minimum frequency ν , called threshold frequency.

ii) Kinetic energy of emitted e^- increases on increasing the frequency but remain unaffected for increasing intensity of light.

But, the classical wave theory of light fails to explain these above observations.

Classical theory was contrary to experimental observations.

Planck had proposed the idea of ene. quantisation but had considered radiation to be a wave.

Einstein used planck's idea of ene. quantisation to explain above mentioned observations.

Einstein proposed that electromagnetic radiation could be considered to have properties of both waves and particles.

He called particles of light as photons.

Each photon of light has ene. equal to $h\nu$.

DATE _____

Now, when light photon of particular frequency hit an electron in metal, it transfers energy $h\nu$ to the electron. The e^- uses this quantum to overcome energy (ω) that binds it in metal and to increase its own kinetic energy ($\frac{1}{2}mv^2$).

$$\therefore h\nu = \omega + \frac{1}{2}mv^2$$

\uparrow B.E. \uparrow K.E.

If $h\nu < \omega \Rightarrow$ no photoelectric effect observed.

As frequency \uparrow K.E. of electron \uparrow
Increase in intensity does not mean \uparrow in K.E. As,
 \uparrow in intensity, \uparrow no. of photons which \uparrow no. of e^- .
and not the kinetic energy.

Electromagnetic radiation then supposed to have a dual character, particle and wave.

$E = mc^2$ Einstein's relativity theory.

$E = h\nu$ Planck's eqⁿ.

$v\lambda = c$ Wave theory of light.

$$\lambda = \frac{c}{\nu} = \frac{h}{mc} = \frac{h}{p}$$

This equation correlates the two properties of a photon. i.e. particle and wave.
as λ , the wavelength is a wave property.
and p , momentum is a particle property.

We have,

$$h\nu = \omega + \frac{1}{2}mv^2$$

$$\therefore \text{K.E. of ejected } e^- \left(\frac{1}{2}mv^2 \right) = h\nu - \omega$$

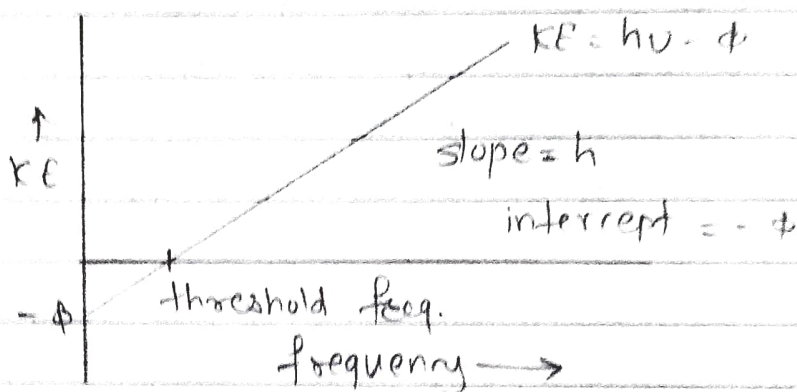
$\omega \rightarrow \phi \rightarrow$ work function

The work function (ϕ) or (ω) is the min. ene. required to remove e^- from surface.

It can be given in terms of threshold frequency -

$$\phi = h\nu_0$$

$$\therefore \text{KE} = h\nu - h\nu_0$$



De Broglie's hypothesis -

Wave-particle duality of material particle.

Louis de Broglie, in 1924 proposed that it was possible to explain quantisation of energy in an atom.

Like electromagnetic light, electrons too exhibit the dual behaviour of particles and waves

$$\lambda = \frac{h}{mv} = \frac{h}{p}$$

Heisenberg's Uncertainty Principle -

To explain the behaviour of electron, Heisenberg (1927) have given a statement -

Simultaneous and accurate determination of position and momentum (velocity) of microscopic particle such as electron is impossible.

If the position is determined accurately the velocity becomes uncertain and vice-versa.

This uncertainty is due to inherent nature (wave-particle duality) of the particle.

Mathematically - $\Delta x \cdot \Delta p_x \approx h$

$$\Delta x = d = \lambda / \sin \theta$$

$$\Delta p_x = p \cdot \sin \theta$$

$$\therefore \Delta x \cdot \Delta p_x = \frac{\lambda}{\sin \theta} \cdot p \sin \theta$$

$$= \lambda \cdot \frac{h}{\lambda} = h$$

$$\Delta x \cdot \Delta p_x \approx h$$

≠ Schrodinger wave equation -

For Hamiltonian operator,

We have eigen equation as -

$$\boxed{\hat{H}\Psi = E\Psi}$$

$$(\hat{K}_x + \hat{V}_x)\Psi = E\Psi$$

$$\left(\frac{\hat{P}_x^2}{2m} + \hat{V}_x\right)\Psi = E\Psi$$

$$\left\{\frac{1}{2m} \left(-i\hbar \frac{d}{dx}\right)^2 + V_x\right\}\Psi = E\Psi$$

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_x\right]\Psi = E\Psi$$

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi + V_x \Psi\right] = E\Psi$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = E\Psi - V_x \Psi$$

$$-\frac{\partial^2 \Psi}{\partial x^2} = \frac{2m}{\hbar^2} (E - V_x) \Psi$$

$$\boxed{\frac{\partial^2 \Psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V_x) \Psi = 0}$$

$$\boxed{\frac{\partial^2 \Psi}{\partial x^2} + \frac{8\pi^2 m}{h^2} (E - V_x) \Psi = 0}$$

$$\dots \hbar = \frac{h}{2\pi}$$

This is Schrodinger wave equation.

Operators -

⇒ Operators are like the mathematical operations addition, subtraction, multiplication.

⇒ As mathematical operations (+ - x) needs numbers to be operated.

Operator needs function / Operand

Some operators and their meanings -

① Position (\hat{x}) ⇒ Multiplication by x .

② Momentum (\hat{P}_x) ⇒ $-i\hbar \frac{d}{dx}$

$$i = i\omega t = \sqrt{-1} \quad \text{and} \quad \hbar = \frac{h}{2\pi}$$

③ Total momentum (\hat{P}) = $\hat{P}_x + \hat{P}_y + \hat{P}_z$
 $= \left(-i\hbar \frac{d}{dx}\right) + \left(-i\hbar \frac{d}{dy}\right) + \left(-i\hbar \frac{d}{dz}\right)$

④ Kinetic energy (\hat{K}_x)

$$K = \frac{1}{2}mv^2 = \frac{1}{2}mv^2 \times \frac{m}{m} = \frac{1}{2} \frac{m^2v^2}{m} = \frac{p^2}{2m}$$

$$\boxed{K = \frac{p^2}{2m}}$$

$$\Rightarrow \hat{K}_x = \frac{\hat{P}_x^2}{2m} = \frac{\left(-i\hbar \frac{d}{dx}\right)^2}{2m} = \frac{-\hbar^2 \frac{d^2}{dx^2}}{2m}$$

⑤ Total kinetic energy (\hat{K})

$$\hat{K} = \hat{K}_x + \hat{K}_y + \hat{K}_z$$

$$= \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) + \left(-\frac{\hbar^2}{2m} \frac{d^2}{dy^2} \right) + \left(-\frac{\hbar^2}{2m} \frac{d^2}{dz^2} \right)$$

⑥ Hamiltonian operator (\hat{H}_x)

↳ Total energy operator. = K.E. + P.E.

$$\hat{H}_x = \hat{K}_x + \hat{V}_x$$

$$\hat{H}_x = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \hat{V}_x$$

⑦ Total Hamiltonian operator. (\hat{H})

$$\hat{H} = \hat{H}_x + \hat{H}_y + \hat{H}_z$$

$$\begin{aligned} \hat{H} &= \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \hat{V}_x \right) + \left(-\frac{\hbar^2}{2m} \frac{d^2}{dy^2} + \hat{V}_y \right) + \left(-\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + \hat{V}_z \right) \\ &= (\hat{K}_x + \hat{V}_x) + (\hat{K}_y + \hat{V}_y) + (\hat{K}_z + \hat{V}_z) \end{aligned}$$

Commutation of an Operator -

⇒ If two operators commute each other then they can be calculated simultaneously.

⇒ Representation of commutation -

$$[\hat{A}, \hat{B}]$$

$$\Rightarrow [\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0 \quad \leftarrow \text{Commutator}$$

then \hat{A} & \hat{B} commute each other.

$$\Rightarrow \hat{A}\hat{B} - \hat{B}\hat{A} = 0$$

$$\boxed{\hat{A}\hat{B} = \hat{B}\hat{A}}$$

Ex. ①. Find the commutator of $\left[\hat{x}, \frac{\hat{d}}{dx}\right]$.

$$\left[\hat{x}, \frac{\hat{d}}{dx}\right] = \left(\hat{x} \cdot \frac{\hat{d}}{dx}\right) - \left(\frac{\hat{d}}{dx} \cdot \hat{x}\right)$$

$$\left[\hat{x}, \frac{\hat{d}}{dx}\right] \psi = \left(\hat{x} \cdot \frac{\hat{d}}{dx} - \frac{\hat{d}}{dx} \cdot \hat{x}\right) \cdot \psi$$

$$= \hat{x} \cdot \frac{\hat{d}}{dx} \psi - \frac{\hat{d}}{dx} \cdot \hat{x} \cdot \psi$$

$$= \hat{x} \cdot \cancel{\frac{\hat{d}}{dx}} \psi - \hat{x} \cdot \cancel{\frac{\hat{d}}{dx}} \psi - \psi \cdot \left(\frac{\hat{d}}{dx} \hat{x}\right)$$

$$= (-1) \psi$$

$$\boxed{\left[\hat{x}, \frac{\hat{d}}{dx}\right] = -1} \quad \leftarrow \text{Commutator}$$

Ex. ② Find the commutator of $\left[\frac{\hat{d}}{dx}, \hat{x}^2 \right]$

Ans. - $\left[\frac{\hat{d}}{dx}, \hat{x}^2 \right] = \left(\frac{\hat{d}}{dx} \hat{x}^2 - \hat{x}^2 \frac{\hat{d}}{dx} \right)$

$$\left[\frac{\hat{d}}{dx}, \hat{x}^2 \right] \psi = \left(\frac{\hat{d}}{dx} \hat{x}^2 - \hat{x}^2 \frac{\hat{d}}{dx} \right) \psi$$

$$= \frac{\hat{d}}{dx} \hat{x}^2 \psi - \hat{x}^2 \frac{\hat{d}}{dx} \psi$$

$$= \hat{x}^2 \cancel{\frac{\hat{d}}{dx}} \psi + \psi \frac{\hat{d}}{dx} \hat{x}^2 - \hat{x}^2 \cancel{\frac{\hat{d}}{dx}} \psi$$

$$= \psi (2x)$$

$$\left[\frac{\hat{d}}{dx}, \hat{x}^2 \right] \psi = (2x) \psi$$

$$\boxed{\left[\frac{\hat{d}}{dx}, \hat{x}^2 \right] = 2x} \rightarrow \text{commutator}$$

Normalisation -

If any wave function ψ satisfies following condition, then it is called as normalised wave function

$$\int \psi^* \psi d\tau = 1$$

→ volume element.

$$\Rightarrow \text{If } \psi = e^{im\phi}$$

$$\text{then } \psi^* = e^{-im\phi}$$

$$\Rightarrow \text{If } \psi = e^{-x^2}$$

$$\text{then } \psi^* = \psi = e^{-x^2}$$

(Change in case of \wedge into only)
sign of.

⇒ Volume element

# Particle in a box	}	1D	⇒	dx
and		2D	⇒	dx · dy
SHO		3D	⇒	dx · dy · dz

$$\# \text{ Rigid Rotor } \left. \vphantom{\int} \right\} \int_0^{2\pi} d\phi$$

Eigen value and Eigen function -

Operator (Function) = constant (Function)

i.e. $\hat{A}\psi = a\psi$ ← Eigen equation

↙ Eigen operator ↘ Eigen function → Eigen value

Que. Find the eigen values :-

1) Operator - $\frac{\hat{d}^2}{dx^2} + 2\frac{\hat{d}}{dx} + 3$

Function - $e^{\alpha x}$

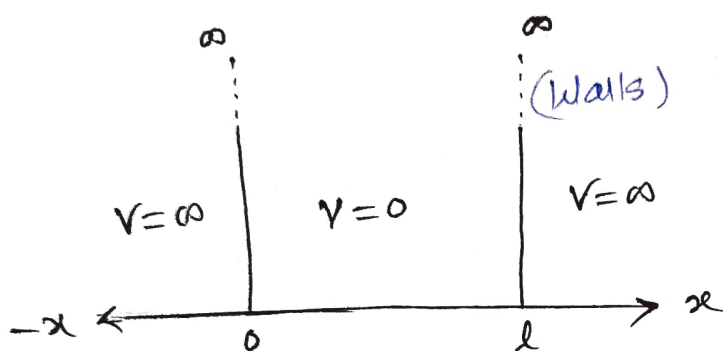
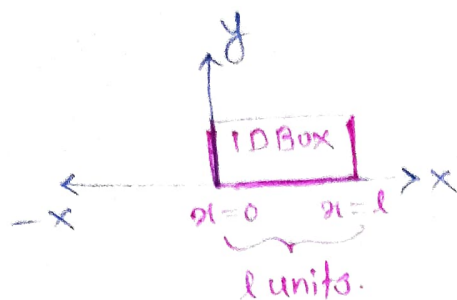
Ans - $\alpha^2 + 2\alpha + 3$

Ans - $\hat{A}\psi = a\psi$

$$\begin{aligned} \left(\frac{\hat{d}^2}{dx^2} + 2\frac{\hat{d}}{dx} + 3 \right) e^{\alpha x} &= \frac{\hat{d}^2}{dx^2} e^{\alpha x} + 2 \cdot \frac{\hat{d}}{dx} e^{\alpha x} + 3 \cdot e^{\alpha x} \\ &= \frac{\hat{d}}{dx} \left(\frac{e^{\alpha x}}{\alpha} \right) \alpha + 2 \cdot \frac{e^{\alpha x}}{\alpha} \alpha + 3 e^{\alpha x} \\ &= e^{\alpha x} \cdot \alpha \cdot \alpha + 2 \cdot e^{\alpha x} \cdot \alpha + 3 e^{\alpha x} \\ &= (\alpha^2 + 2\alpha + 3) \cdot e^{\alpha x} \end{aligned}$$

⇒ $\boxed{\text{Eigen value} = \alpha^2 + 2\alpha + 3}$

Particle in a 1-D Box -



⇒ ∞ walls means particle cannot go outside the box.

⇒ Wave function of a particle -

$$\psi = \sqrt{\frac{2}{l}} \cdot \sin\left(\frac{n\pi x}{l}\right)$$

⇒ Particle will be present inside the box.
To check - whether particle is present on walls or not
Boundary -

$$x=0 \Rightarrow \psi = \sqrt{\frac{2}{l}} \cdot \sin 0^\circ \Rightarrow \boxed{\psi = 0}$$

$$x=l \Rightarrow \psi = \sqrt{\frac{2}{l}} \cdot \sin(n\pi)$$

$$\Rightarrow \boxed{\psi = 0}$$

↪ particle does not exist

⇒ Particle does not exist on walls.

Particle is a free particle.

That means - There is no other particle inside the box.

That means - There will be no any force on that free particle.

$$F = -\frac{dV}{dx}$$

⇒ No potential also inside in box.

⇒ Outside the box, there will be particles in environment
Hence $V = \infty$

For 1D Box - Remember -

$$\Psi(x) = \sqrt{\frac{2}{l}} \cdot \sin\left(\frac{n\pi x}{l}\right)$$

$$E = \frac{n^2 h^2}{8ml^2}$$

$$n = 1, 2, 3, 4, \dots, \infty$$

$$n \neq 0$$

→ mass of particle.

Wave function plots - **1D Box**

$$\Psi = \sqrt{\frac{2}{l}} \cdot \sin\left(\frac{n\pi x}{l}\right)$$

Ground State (n=1)

$$\Psi_1 = \sqrt{\frac{2}{l}} \cdot \sin\left(\frac{\pi x}{l}\right)$$

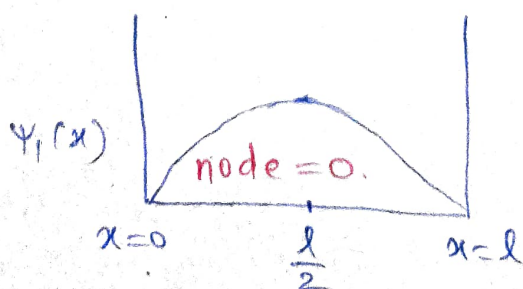
⇒ For Ψ_1 to be maximum, term of \sin must be max.
Max. value of \sin function is 1.

$$\sin\frac{\pi x}{l} = 1 \rightarrow \sin\frac{\pi}{2}$$

$$\sin\frac{\pi x}{l} = \sin\frac{\pi}{2}$$

$$\frac{x}{l} = \frac{1}{2}$$

$$x = l/2$$



Transition Dipole Moment Integral -

Transition probability -
probability of particular spectroscopic transition to take place.

It depends on -

- i) Nature of initial & final state wavefunctions.
- ii) How strongly photons interact with an eigenstate

Selection rules are utilized to determine whether a transition is allowed or not.

- i) Electronic selection rules
- ii) Vibrational selection rules
- iii) Rotational selection rules

Transition Moment -

In atom, electromagnetic wave can induce oscillating electric or magnetic moment.

If the freq. of induced electric or magnetic moment is same as the ene. difference between one eigenstate ψ_1 and another ψ_2 ,

the interaction between an atom or molecule and the electromagnetic field is resonant.

(means these two have same frequency)

The amplitude of this moment is called the transition moment.

from ψ_1 to ψ_2

Transition dipole moment / transition moment (\vec{M}_{21})

Transition probability ($|\vec{M}_{21}|^2$)

Mathematically,

$$\vec{M}_{01} = \int \Psi_2 \vec{\mu} \Psi_1 d\tau$$

μ is the dipole moment operator.

If system have n molecules and each has charge Q_n .

$$\vec{\mu} = \sum_n Q_n \cdot \vec{r}_n$$

↑ position vector operator.

Transition moment integral -

Born Oppenheimer approximation -

The fast electronic motion can be separated from much slower motion of nuclei.

Therefore,

The total wavefunction can be separated into electronic, vibrational and rotational parts -

$$\Psi(r, R) = \Psi_e(r, R_e) \Psi_v(R) \Psi_r(R)$$

Since mass of electrons is much smaller than nuclear mass, the rotational wavefunction, Ψ_r , only depends on nuclear co-ordinates.

With rotational part removed, transition moment integral can be expressed as -

Both the nuclear and electronic parts contribute to the dipole moment operator. The above eqⁿ can be integrated by two parts with μ_n and μ_e resp.

A product of two integral is obtained.

$$M = \int \Psi_e'(r, R_e) \cdot \mu_e \Psi_e''(r, R_e) dr \int \Psi_v'(R) \Psi_v''(R) dR + \int \Psi_v'(R) \cdot \mu_n \Psi_v''(R) dR \int \Psi_e'(r, R_e) \Psi_e''(r, R_e) R dr$$

Because different electronic wavefunctions must be orthogonal to each other

Hence, $\int \Psi_e'(r, R_e) \Psi_e''(r, R_e) dr = 0$

\therefore Second part of integral should be zero.

\therefore Transition moment integral can be simplified as

$$M = \int \Psi_e'(r, R_e) \cdot \mu_e \Psi_e''(r, R_e) dr \int \Psi_v'(R) \Psi_v''(R) dR$$

Above equation is of great importance 'cause first integral defines electronic selection rules, while the second integral is the

Rotational Selection Rules-

① Transitions with $\Delta J = \pm 1$ are allowed.

Photons do not have any mass, but they have angular momentum.

The conservation of angular momentum is fundamental criteria for spectroscopic transitions.

The rotational selection rules relies on the fact that photon has one unit of quantized angular momentum.

During the photon emission and absorption process, angular momentum J cannot change by more than ± 1 unit.

$$\Delta J = +1 \quad \leftarrow \quad \text{R Branch}$$

$$\Delta J = -1 \quad \leftarrow \quad \text{P Branch}$$

② $\Delta J = 0$ transitions are allowed when two different electronic or vibrational states are involved.

$$(x'', J'' = m) \rightarrow (x', J' = m)$$

$$\Delta J = 0 \quad \leftarrow \quad \text{Q Branch}$$

Q branch transition will only take place when there is net orbital angular momentum in one of the electronic states.

Q branch does not exist for ${}^1\Sigma \leftrightarrow {}^1\Sigma$ electronic transition because Σ electronic state doesn't possess net orbital angular momentum.

Q branch will exist if one of the electronic states has angular momentum.

For polyatomic molecule - $\Delta K = 0$.
with symmetric top geometry. Selection rule.

Electronic Selection Rules -

① In Atoms -

Atoms are described by

n - primary quantum number

L - angular momentum quantum number

S - spin quantum number

J - total angular momentum quantum number

Based on Russell - Saunders approx. of coupling -

Atomic term symbol - $2s+1 L_J$

1. The total spin cannot change. ($\Delta S = 0$)
2. Change in total orbital angular momentum can be $\Delta L = 0, \pm 1$.

But $L=0 \leftrightarrow L=0$ transition is not allowed.

3. $\Delta J = 0, \pm 1$. But $J=0 \leftrightarrow J=0$ is not allowed
4. Initial and final wavefunctions must change in parity
 even \leftrightarrow odd transitions are allowed.

② In Molecules -

Electronic - state configurations for molecules are described by

n - primary quantum no.

Λ - angular momentum quantum no.

S - Spin quantum no.

Term symbol -

$2S+1 \Lambda^{(+/-)}_{\Sigma, (\pi, \sigma)}$

1. $\Delta S = 0$.

rule $\Delta E = 0$ holds for multiplets

2. $\Delta l = 0, \pm 1$

For heteronuclear diatomic molecule with $C_{\infty v}$ symmetry

$\Sigma^+ \leftrightarrow \pi$ transition is allowed.

3. For homonuclear molecules -

$g \leftrightarrow u$ transition is allowed.

For heteronuclear molecules -

$+ \leftrightarrow +$ and $- \leftrightarrow -$ transitions apply.

Vibrational Selection Rules-

1. $\Delta v = \pm 1, \pm 2, \dots$ are allowed. For anharmonic potential

But intensity of peaks become weaker as $\Delta v \uparrow$.

2. $v=0 \rightarrow v=1 \Rightarrow$ Fundamental vibration.

Others are overtones.

3. $\Delta v = 0$ transition is allowed bet. lower & upper electronic states with energy E_1 and E_2 involved.

Vibrational selection rules does not exist for diatomic m.
Frank-Condon integral is always totally symmetric for diatomic molecules.

For polyatomic \rightarrow Non-linear $\rightarrow 3N - 6$ vibrational modes.

linear $\rightarrow 3N - 5$ vibrational modes.

Based on harmonic oscillator model, the product of $3N - 6$ normal mode wavefunctions contribute to total vibrational wavefunction. i.e.

$$\Psi_{vib} = \prod_{3N-6} \psi_1 \psi_2 \psi_3 \dots \psi_{3N-6}$$

Angular momentum

Angular momentum = position \times momentum

$$L = r \times p$$

↳ linear momentum

$$\hat{L} = \hat{r} \otimes \hat{p}$$

↳ cross product (vectors)

Cross product -

$$(\alpha \hat{i} + y \hat{j} + z \hat{k}) \times (m \hat{i} + n \hat{j} + l \hat{k})$$

$$= \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \alpha & y & z \\ m & n & l \end{vmatrix}$$

$$= i(yl - nz) - j(\alpha l - zm) + k(\alpha n - ym)$$

Now, $\hat{r} = \hat{x} \hat{i} + \hat{y} \hat{j} + \hat{z} \hat{k}$

$$\hat{p} = \hat{p}_x \hat{i} + \hat{p}_y \hat{j} + \hat{p}_z \hat{k}$$

$$\hat{r} \times \hat{p} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \hat{x} & \hat{y} & \hat{z} \\ \hat{p}_x & \hat{p}_y & \hat{p}_z \end{vmatrix}$$

$$= (\hat{y} \cdot \hat{p}_z - \hat{z} \cdot \hat{p}_y) \hat{i} - (\hat{x} \cdot \hat{p}_z - \hat{z} \cdot \hat{p}_x) \hat{j} + (\hat{x} \cdot \hat{p}_y - \hat{y} \cdot \hat{p}_x) \hat{k}$$

Total angular momentum -

$$\hat{L} = \hat{L}_x \cdot \hat{i} + \hat{L}_y \cdot \hat{j} + \hat{L}_z \cdot \hat{k}$$