Chaitanya Kapoor
2020A3PS1219P
f20201219@pilani.bits-pilani.ac.in

General Chemistry

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Some useful constants:

- h (Planck's constant) $= 6.626 \times 10^{-34}$ J-s
- c (Speed of light) $= 2.998 \times 10^{8} \approx 3 \times 10^{8}$ m/s
- m_e (Mass of electron) $= 9.1 \times 10^{-31}$ kg
- e (Charge on an electron) $= 1.6 \times 10^{-19}$ C
- $\hbar$ (Reduced Planck's constant) $= 1.055 \times 10^{-34}$ J-s

1 Photoelectric effect

- Let the frequency of the incident light on the metal surface be ν, and the work function of the metal be ϕ. The energy of the ejected photon is given by:

  $$E = h\nu - \phi$$

  Which can be rewritten in terms of the wavelength (λ) and the speed of light (c) as:

  $$E = \frac{hc}{\lambda} - \phi$$

  In the case where

  $$\phi = h\nu_0 = \frac{hc}{\lambda_0}$$

  ν_0 and λ_0 are called the **threshold frequency and wavelength** respectively.

- For a particle of mass m travelling with a velocity v, its (De Broglie) wavelength takes the form:

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

  Where p is the linear momentum of the particle in question.

- When an electron of charge $-e$ is accelerated across a potential difference V, it acquires the kinetic energy $E = eV$. From this, it follows that the *De Broglie wavelength* of the particle is:

  $$\lambda = \frac{h}{\sqrt{2m_e eV}}$$

  m_e being the mass of the electron.

2 Schrödinger equation

- The **time independent Schrödinger equation** for a particle having the wavefunction ψ (in a single dimension) is

  $$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

  The left hand side of the above equation is abbreviated to a *single operator* known as the **Hamiltonian**, which represents the **total energy of a particular system**. We now have a compact version of the S.E: $\boxed{\hat{H}\psi = E\psi}$

- A wavefunction ψ is said to be **normalised** if its probability density over the entire space is 1. More formally, the following relation must hold

  $$\int_{-\infty}^{\infty} \psi^* \psi dx = 1$$

  Where ψ^* is the **complex conjugate** of ψ. Note that *psi* is normalized only for a 1 dimensional case above.

- Suppose that Δx and Δp denotes the uncertainty in the measurement of position and momentum respectively. Heisenberg's uncertainty principle states

  $$\Delta x \Delta p \geq \frac{\hbar}{2}$$

3 Particle In a Box

1. **1D case**:
   We consider a box of length L, quantum number n, particle mass m and wavelength of the particle λ

   - Acceptable values of linear momentum $p = \frac{nh}{2L}$
   - Solution to the Schrödinger equation for the n^{th} excited state:

   $$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

   - Permitted energy values:

   $$E_n = \frac{n^2 h^2}{8mL^2}$$

     The energy of the lowest state ($n = 1$) is called the **zero-point energy**

2. **2D case**:
   A box of dimensions L_x and L_y along the x and y directions is considered, with the quantum numbers n_x and n_y

   - Solution to the Schrödinger equation:

   $$\psi_{n_x n_y}(x, y) = \sqrt{\left(\frac{4}{L_x L_y}\right)} \sin\left(\frac{n_x \pi x}{L_x}\right) \sin\left(\frac{n_y \pi y}{L_y}\right)$$

   - Permissible energy values:

   $$E_{n_x n_y} = \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2}\right) \frac{h^2}{8m}$$

4 Rigid Rotor

1. **2D case**:
   We consider here a particle of mass m rotating in a circle of radius r. The moment of inertia of the system is taken to be $I = mr^2$

   - Angular momentum $J_z = m_l \hbar$ where $m_l = 0, \pm 1, \pm 2 \ldots$
   - Permissible energy values $E_n = \frac{n^2 \hbar^2}{2I} = \frac{m_l^2 \hbar^2}{2I}$ where m_l and $n = 0, \pm 1, \pm 2 \ldots$

2. **3D case**:
   In addition to the previously defined quantities, we introduce l: the **orbital angular momentum quantum number**.

   - Permissible energy values $E_l = l(l+1)\frac{\hbar^2}{2mr^2}$
     Here, $l = 0, 1, 2 \ldots$ and $m_l = -l, (-l+1) \ldots (l-1), l$
   - Angular momentum is **quantized** and given by the values $J = \sqrt{l(l+1)}\hbar$

5 Simple Harmonic Oscillator

Here, we are concerned only with the permissible energy values:

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

Where ν is the **vibrational frequency** given by $\frac{1}{2\pi}\sqrt{\frac{k}{m}}$. The values of ν include the set of all non-negative integers.