SUBJECT - CHEMISTRY
CLASS - B.Sc(Hons) PART-III
PAPER - V
TOPIC. Zero point energy
Dr Hari Mohan prasad Singh
Department of chemistry
Dr. L.K.V.D College Tajpur Samastipur

Q Show that occurrence of Zero Point energy is in accordance with Heisenberg uncertainty principle.

Ans The energy of a particle in one dimensional box is given by —

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

Although Zero value of n is permitted but it is not acceptable because then ψ becomes Zero while an electron is assumed to be always present inside the box. Therefore lowest Kinetic energy called Zero point energy of an electron in a box is given by putting $n = 1$ i.e

$$E_0 = \frac{h^2}{8mL^2}$$

This shows that the electron inside the box is not at rest event at 0°K Hence the position of electron cannot be precisely known. Thus the occurence of Zero point energy is in accordance with Heisenberg uncertainty principle.

Q Show that a particle in a one-dimensional box cannot have a definitely known momentum and that the average value of the momentum is zero

Ans for a particle in a one dimensional box of length L, we have –

$$\psi = \sqrt{2/L}\ \sin \frac{n\pi}{L}.x \quad \text{where } n = 1, 2, 3 \cdots$$

$$\therefore\ \bar{P}_x = \int_0^L \psi^* \left(\frac{h}{2\pi i} \cdot \frac{\partial}{\partial x}\right) \psi dx$$

$$= \frac{h}{2\pi i} \cdot \frac{2}{L} \int_0^L \sin \frac{n\pi}{L}.x . \cos \frac{n\pi}{L}.x\ \frac{n\pi}{L}.dx$$

$$= \frac{h}{\pi i} \cdot \frac{n\pi}{L2} \int_0^L \sin \frac{2n\pi}{l} x\, dx$$

$$= \frac{h}{\pi i} \cdot \frac{n\pi}{L2} \times 0 = 0$$

$$\bar{P}_x^2 = \int_0^L \psi^* \left(-\frac{h^2}{4\pi^2} \frac{\partial^2}{\partial x^2}\right) \psi\, dx = \frac{h^2 n^2}{4L^2}$$

Hence the mean deviation $\bar{P_x^2} - (\bar{P}_x)^2 \neq 0$

Hence px is not definitely known