

ESR spectroscopy ①

Electron spin resonance or electron paramagnetic resonance spectroscopy (EPR) is a method for studying materials with unpaired electrons. The basic concepts of ESR similar to those of nuclear magnetic resonance, but here the electron spin ~~are~~ that are excited instead of the spins of atomic nuclei.

Theory or basic principle:- The presence of an unpaired electron in a molecule or ion allows energy levels to be produced from the interaction of the magnetic moment of the electron with an applied magnetic field.

Every electron has a magnetic moment and spin quantum number $S = \frac{1}{2}$, with magnetic components $m_s = +\frac{1}{2}$ or $m_s = -\frac{1}{2}$, in the presence of an external magnetic field, with strength B_0 . The electronic magnetic moment aligns itself either parallel ($m_s = +\frac{1}{2}$) or antiparallel ($m_s = -\frac{1}{2}$) to the field.

In ESR spectra, a transition between the different electron spin energy states (due to the presence of an applied magnetic field) occurs upon absorption of a photon.

(ii)
Quantum of radiation in microwave region.

The energy difference between the two states is given by

$$\Delta E = h\nu = g_e \mu_B B_0$$

for unpaired free electrons.

Where g_e is called g -factor (Lande g factor). Its value is 2.0023 for the free electron.

μ_B = Bohr magneton.

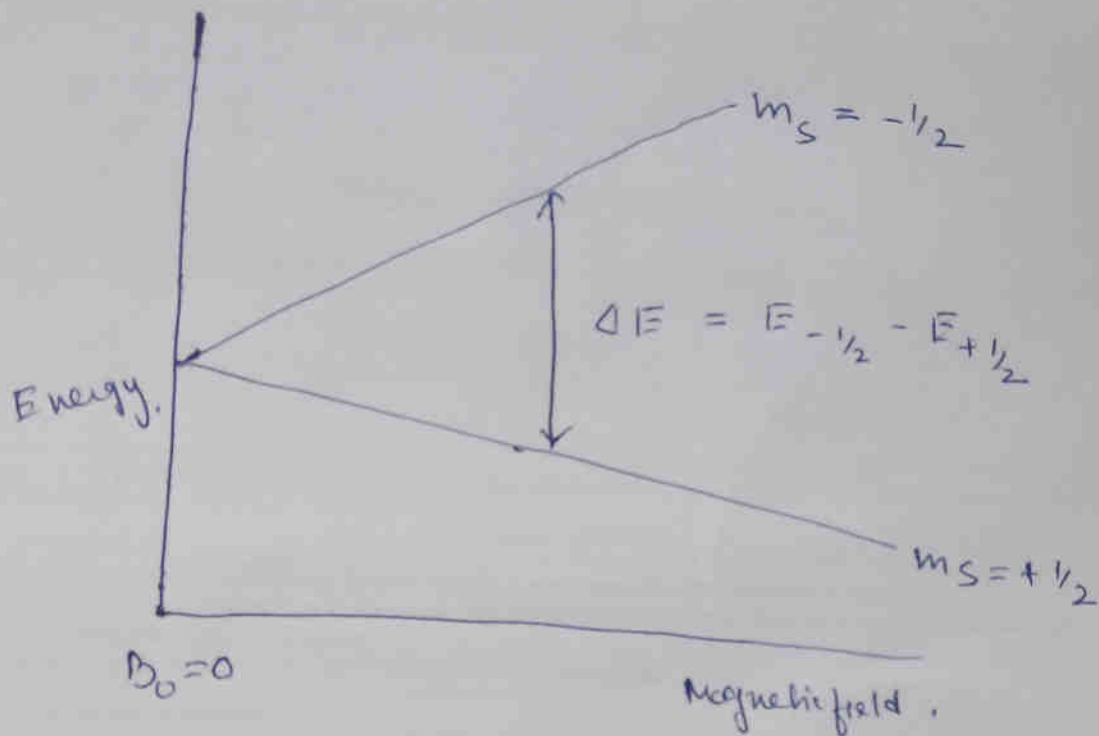
B_0 = Magnetic field.

The quantity g_e (also called spectroscopic splitting factor) is not constant and depends upon the orientation of the molecules containing the ~~the~~ unpaired electrons with respect to the magnetic field. The value of g_e also depends upon the states of the sample (e.g. gas, liquid or solid). μ_B is constant. So in this case splitting of energy level is directly proportional to the magnetic field strength as shown in the diagram.

An unpaired electron can move between the two energy levels by absorbing or emitting a photon of energy $h\nu$ such that the resonance

(III).

Condition $h\nu = \Delta E$ is obeyed. This leads to the fundamental equation of ESR spectroscopy $\Delta E = h\nu = g_e \mu_B B_0$.



Q: Why ESR transition occurs in the microwave region and NMR transition in radio frequency region?

Ans: The electron spin magnetic moment is about a thousand times greater than magnetic moment of nucleus. The energy of interaction of the magnetic moment of unpaired electron with the applied field will be greater than the corresponding interaction between nuclear magnetic moment and the applied field. So ESR transition occurs in microwave region and NMR in radio wave region.