

Full Form-EPR (Electron Paramagnetic Resonance)



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Introduction:

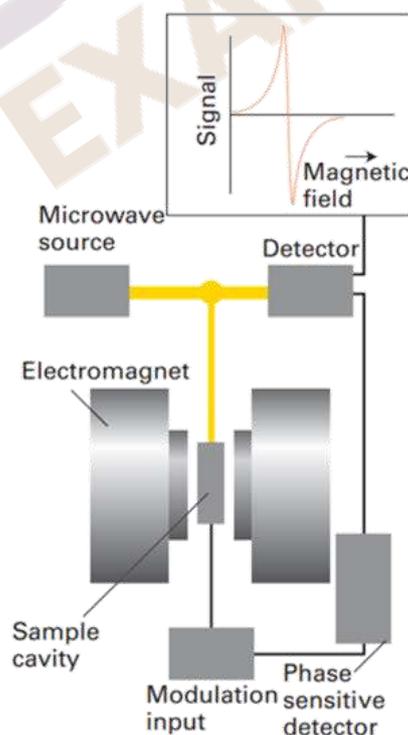
Electron paramagnetic resonance spectroscopy is used to study those compounds that contain unpaired electrons, particularly those containing a d-block element. It is also considered as a technique to identify and study metals such as Fe and Cu at the active sites of metalloenzymes. In the case of a magnetic field, EPR is used to study paramagnetic species such as organic and main-group radicals. In inorganic chemistry, its main principle is to characterize compounds containing the d- and f-block elements.

In the simplest case of species containing one unpaired electron, the application of an external magnetic field B_0 produces a difference in energy between the $m_s = +\frac{1}{2}$ and $m_s = -\frac{1}{2}$ states of the electron, with $\Delta E = g\mu_B B_0$

Here, μ_B is the Bohr magneton and g is a numerical factor known simply as the g value.

Types:

Continuous Wave Spectrometer: To record the EPR spectra, the conventional method is to use a continuous wave (CW) spectrometer in which the irradiation of the sample with a constant microwave frequency takes place and the applied magnetic field is varied.



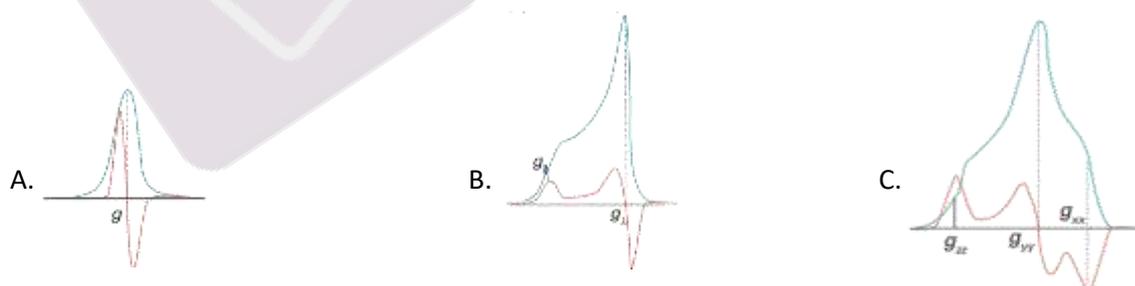
The layout of a typical continuous wave EPR spectrometer.

X-Band Spectrometer: For most of the spectrometers, the resonance frequency is approximately around 9 GHz, and this instrument is known as an 'X-band spectrometer'. The magnetic field in this spectrometer is about 0.3 T. Laboratories that are specialized in EPR spectroscopy often have a range of instruments, each operating at different fields. Thus, an S-band having a resonant frequency 3 GHz spectrometer and particularly those operating at high fields, Q-band (35 GHz) and W-band (95 GHz) spectrometers, are used to complement the information gained with an X-band spectrometer.

Pulsed EPR Spectrometers: These spectrometers are now commercially available and tend to offer new opportunities that are like the way that pulsed Fourier-transform techniques have revolutionized NMR. Techniques used by this spectrometer provide time resolution which makes the measure of dynamic properties of paramagnetic systems possible.

Different Terminologies:

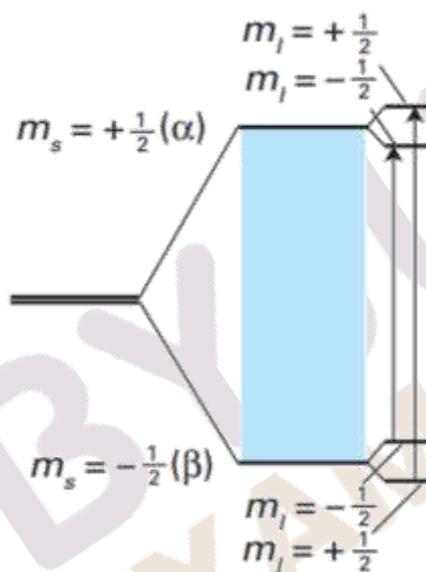
The g value: For a free electron, the value of g is 2.0023 but this value gets altered by spin-orbit coupling which changes the local magnetic field experienced by the electron. For many species particularly of d-metal complexes, g value can be highly anisotropic. Due to this, resonance condition depends on the angle that the paramagnetic species makes to the applied field. The sample which is present in a quartz tube comprises the paramagnetic species in dilute form, either in the solid state (doped crystals or powders) or in solution. Frozen solutions generally behave like an amorphous powder, as a result, resonances can be observed at all the g values of the compound, analogous to powder X-ray diffraction. For systems having more than one unpaired electron, spectra can be obtained such as triplet states, but the theoretical background is much more complicated. Species containing an odd number of electrons can be detected but it is difficult to observe spectra for systems having an even number of electrons.



The above representation shows the forms of EPR powder (frozen solution) spectra expected for different types of g value anisotropy. The green line represents the absorption while the red line represents the first derivative of the absorption (its slope).

Hyperfine coupling: In an EPR spectrum, the hyperfine structure is formed due to the coupling of the electron spin to any magnetic nuclei present. A nucleus of spin I splits an EPR line into $2I + 1$ lines of the same intensity. Sometimes, a distinction can be made between the hyperfine structure due to coupling with the nucleus of the atom which contains the unpaired electron and the 'super hyperfine coupling, the coupling to ligand nuclei. This coupling measures the extent of electron delocalization and covalence in metal complexes.

In the presence of a magnetic field, $2I+1$ orientations give rise to a local magnetic field that splits each spin state of an electron into $2I + 1$ levels. The allowed transitions ($\Delta m_s = +1, \Delta m_l = 0$) gives rise to the hyperfine structure of an EPR spectrum.



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