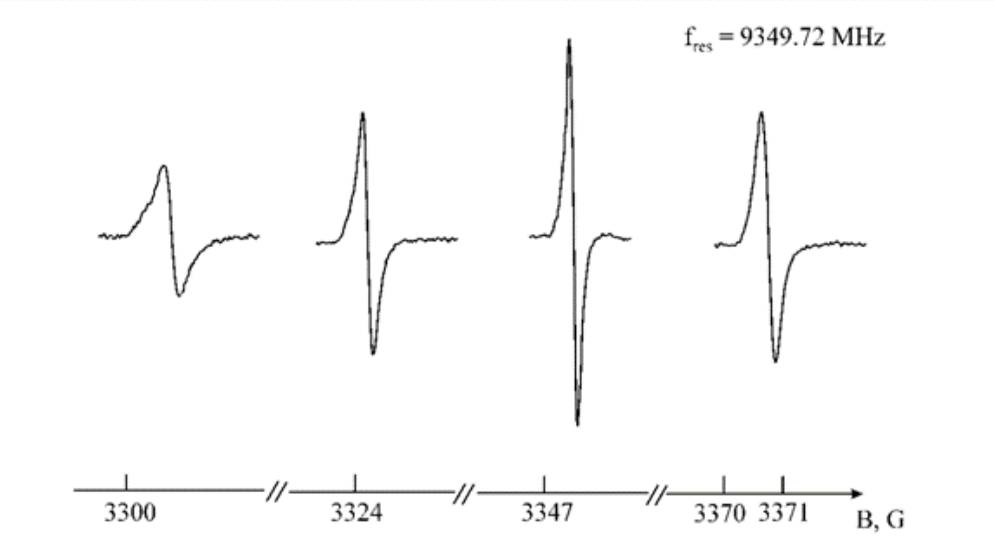
APPLICATIONS OF ESR SPECTROSCOPY



Dr. M. KALANITHI,

ASSOCIATE PROFESSOR OF CHEMISTRY,

JAYARAJ ANNAPACKIAM COLLEGE FOR WOMEN,

PERIYAKULAM

ELECTRON SPIN RESONANCE (ESR)

- It is a branch of absorption spectroscopy.
- It occurs in long wavelength region of microwaves
- It requires 0.5 T of applied magnetic field
- Magnetic energy splitting is done by applying a static magnetic field.

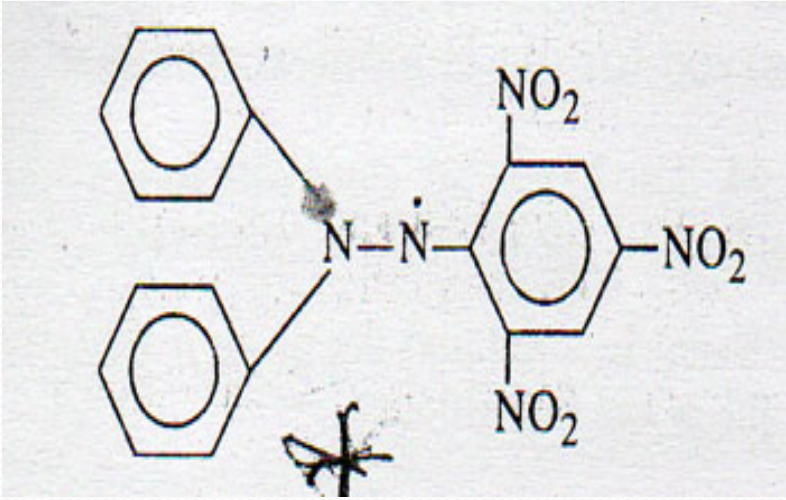
Applications of ESR

- Determination of the structure of organic and inorganic free radicals.
- These radicals may be produced chemically , photo chemically or by using high-energy radiation.
- The free radicals are very short-lived, they are trapped in a glasses, frozen rare-gas matrices or in crystals.
- The free radical must be produced in a concentration of about 10^{-13} mol dm^{-3}.

CONT……

- The intensity of an ESR signal is directly proportional to the number of the free radical present.
- It can be used to measure the relative concentrations of free radicals produced under different conditions .
- Hyperfine interaction in ESR spectra can provide useful information about charge distribution within a molecule .

CONT…..



DPPH – α, α’ diphenylpicrylhydrazyl radical

It gives five extremely sharp peaks with intensity ratio 1 : 2 : 3 : 2 :1 in the ESR spectrum.

CONT.....

The difference between a triplet state molecule and a diradical,

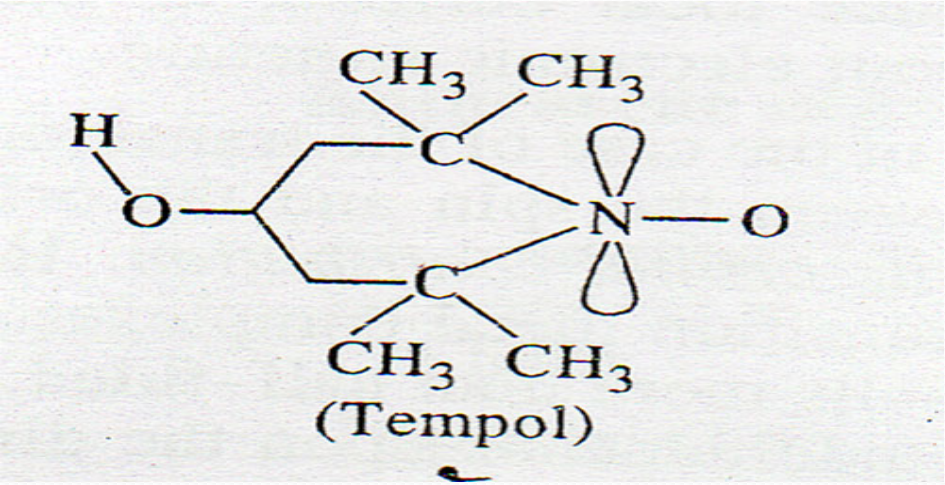
- Both contains two unpaired electrons
- In a **triplet state molecule**, the **unpaired electrons must interact.**
- In a **diradical**, the unpaired electrons **do not interact for their great distance.**

CONT.....

H.M. McConnell and his Co-workers found that,

- The groups with unpaired electrons can be attached to macromolecules such as proteins and membranes.
- The nitroxide molecules bound to macromolecules - **Spin labels**.
- These are stable molecules - unpaired 2p electrons.

CONT…..



2,2,6, 6 – tetramethyl piperidinol-N-oxyl

CONT……

- The hyperfine structure of an ESR spectrum is a kind of finger print – helps to identify the free radicals present in the sample.

THANK YOU