EPR Spectra

ESR Electron Spin Resonance

EPR Electron Paramagnetic Resonance

The EPR spectra are mainly acquired in CW mode

CW (continuous wave) Signal

- The signal is observed in the presence of a low power r.f. magnetic field, B_1, as a function of the r.f. frequency
- The signal is obtained as a function of frequency
- B^r magnetic field in the rotating frame
- The y' axis is chosen for the r.f. magnetic field

$$B^r = \begin{vmatrix} 0 \\ -\dfrac{\omega_1}{\gamma} \\ -\dfrac{\Omega_0}{\gamma} \end{vmatrix}$$

For this system the Bloch equations are:

$$\frac{dM_x}{dt} = \gamma\left(M_y B_z - M_z B_y\right) - \frac{M_x}{T_2} = -\Omega M_y + \omega_1 M_z - \frac{M_x}{T_2}$$

$$\frac{dM_y}{dt} = \gamma\left(M_z B_x - M_x B_z\right) = \Omega M_x - \frac{M_y}{T_2}$$

$$\frac{dM_z}{dt} = \gamma\left(M_x B_y - M_y B_x\right) - \frac{M_z - M_0}{T_1} = -\omega_1 M_x - \frac{M_z - M_0}{T_1}$$

The solution are looked for at the *steady state*

$$\frac{dM_x}{dt} = 0 \qquad \frac{dM_y}{dt} = 0 \qquad \frac{dM_z}{dt} = 0$$

Thus we must solve a systems of three equations with three unknowns

$$-\Omega M_y + \omega_1 M_z - \frac{M_x}{T_2} = 0$$

$$\Omega M_x - \frac{M_y}{T_2} = 0$$

$$-\omega_1 M_x - \frac{M_z - M_0}{T_2} = 0$$

M_x, obtained from the second equation, is used in the third one

$$-\frac{\omega_1 M_y}{\Omega T_2} - \frac{M_z}{T_1} + \frac{M_0}{T_1} = 0$$

M_z is obtained as: $M_z = M_0 - \frac{T_1 \omega_1 M_y}{\Omega T_2}$

Substituting for M_z e M_x in the first equation:

$$-\Omega M_y + \omega_1 M_0 - \frac{T_1 \omega_1^2 M_y}{\Omega T_2} - \frac{M_y}{\Omega T_2{}^2} = 0 \qquad / \cdot \Omega T_2^2$$

$$-\Omega^2 T_2^2 M_y + \omega_1 \Omega T_2^2 M_0 - T_1 T_2 \omega_1^2 M_y - M_y = 0$$

$$M_y \left(1 + \Omega^2 T_2^2 + \omega_1^2 T_1 T_2 \right) = \omega_1 \Omega T_1 T_2$$

$$\boxed{M_y = \omega_1 M_0 \frac{\Omega T_2^2}{1+\Omega^2 T_2^2 + \omega_1^2 T_1 T_2}}$$

Dispersion

Since: $$M_x = \frac{M_y}{\Omega T_2}$$

$$\boxed{M_x = \omega_1 M_0 \frac{T_2}{1+\Omega^2 T_2^2 + \omega_1^2 T_1 T_2}}$$

Absorption

Under **non saturation** conditions, that is: $\omega_1^2 T_1 T_2 << 1$ it can be neglected, and the lineshape is **Lorentzian**

First Derivative

$$y = c\frac{1}{a + bx^2}$$

$$\frac{dy}{dx} = -c\frac{2bx}{(a + bx^2)^2}$$