

Electron Spin Resonance Spectroscopy

Calculating Landè g factor

Ravitej Uppu

Aim

To find the value of the Landè g factor for an electron subjected to a perturbation by an external alternating magnetic field.

1 Theory

Electron spin resonance (ESR) is a useful tool for investigating the energy absorption spectra of many materials with unpaired electrons (paramagnetic materials). The molecule will have an intrinsic magnetic dipole moment due to the unpaired electron. ESR is a purely quantum mechanical effect. It relates the interaction of an external magnetic field to an electron's magnetic moment, which is a result of its intrinsic spin. Since the spin of an electron may either be up or down, so may its magnetic moment. This implies that, in the presence of an external magnetic field, one spin state will be higher in energy than the other. The spin with a moment pointing in the direction of the external field is lowest in energy. These states have an energy E , as

$$E = \pm \frac{1}{2} g \mu_B B$$

where μ_B is the Bohr Magneton and B , the external Magnetic field. Hence, the change in energy from the negative spin state to positive spin state is

$$\Delta E = g \mu_B B$$

At commonly attainable magnetic field strengths the corresponding energy lies in the radio-frequency (RF) regime. Where the general expression for the energy of a photon applies and we have

$$\Delta E = h(\nu_1 - \nu_2)$$

An unpaired electron responds not only to a spectrometer's applied magnetic field B_0 , but also to any local magnetic fields of atoms or molecules.

The effective field B_{eff} experienced by an electron is thus written $B_{eff} = B_0(1 - \sigma)$, where σ includes the effects of the local fields. Hence, resonance condition can be written as

$$h\nu = g_e\mu_B B_{eff} = g_e\mu_B B_0(1 - \sigma) = g\mu_B B_0$$

where g_e is the electron's g -factor and we have used the relation between σ and g to get the last form.

This last equation is used to determine g in this experiment by measuring the field and the frequency at which resonance occurs. If g does not equal g_e , the implication is that the ratio of the unpaired electron's spin magnetic moment to its angular momentum differs from the free electron value. Since an electron's spin magnetic moment is constant (approximately the Bohr magneton), then the electron must have gained or lost angular momentum through spin-orbit coupling. Because the mechanisms of spin-orbit coupling are well understood, the magnitude of the change gives information about the nature of the atomic or molecular orbital containing the unpaired electron.

2 Procedure

The electrons that you will manipulate are located in the paramagnetic molecule Diphenyl-Picryl-Hydrazyl (DPPH). The free electron is also very weakly bound to the nitrogen atom. This molecule ideal for studying the magnetic properties of the electron. The sample is placed in a tube and is placed between the Helmholtz coils. After completing the necessary circuit which majorly consists of two parts, one for monitoring the frequency of RF oscillator and the other for controlling external Magnetic Field (B); we also have an oscilloscope for making the necessary measurements. We observe the output of the absorption of the DPPH on one channel of the oscilloscope and the voltage across the resistor (internal) on the other channel. The measurements are made in the X-Y mode.

Now, we fix arbitrarily choose a position for the the frequency knob, set sensitivity to full, and set current to a value near $100mA$. Then, we adjust the phase such of the four observed peaks, there is a match in a set of two peaks. Now, we use the RF-Oscillator to check for the resonance and determine approximately the set value of the frequency. From this, and from the distance between the two peaks ($2Q$) and width of plot P we calculate the magnetic field H as well as H_0 . From this, we can approximately get the value of g from the last relation of the previous section. Some of the relation used here are,

$$H = \frac{32\pi n}{10\sqrt{125}a} I$$

$$H_0 = \frac{2\sqrt{2}HQ}{P} \text{ gauss}$$

$$\Rightarrow QI = \frac{Ph\nu_0 10\sqrt{(125)a}}{64\sqrt{2}\mu_0\pi n} \frac{1}{g}$$

where n are the number of turns in each coil, a is the radius of the coil, I is the current flowing in the coils and ν_0 is the frequency of the magnetic field.

For better results, i.e. to remove any random errors it is better to plot a $1/I$ versus Q graph, get the slope and from that we can use the QI relation to get the value of g .

3 Observations and Results

- $n = 500$
- $a = 7.7\text{cm}$
- For $\nu_0 = 11.25\text{MHz}$,
 - $I = 100\text{mA}$
 - $P = 26\text{V}$
 - $2Q = 13\text{V}$
 - $H = 5.84\text{gauss}$
 - $H_0 = 4.13\text{gauss}$
 - $g_{\text{calculated}} = 1.95$
 - slope of $1/I$ versus Q graph is = 1.27
- For $\nu_0 = 13.5\text{MHz}$,
 - $I = 125\text{mA}$
 - $P = 32\text{V}$
 - $2Q = 15.2\text{V}$
 - $H = 7.30\text{gauss}$
 - $H_0 = 4.90\text{gauss}$
 - $g_{\text{calculated}} = 1.97$
 - slope of $1/I$ versus Q graph is = 1.87

- Data obtained by varying current and getting the $2Q$ from the oscilloscope screen for $\nu_0 = 11.25MHz$

S.No	$I(mA)$	$2Q V$	$Q V$	$1/I A^{-1}$
1	100	13.0	6.5	10.00
2	125	10.4	5.2	8.00
3	175	7.4	3.7	5.71
4	200	6.6	3.3	5.00
5	230	5.6	2.8	4.35

- Data obtained by varying current and getting the $2Q$ from the oscilloscope screen for $\nu_0 = 13.5MHz$

S.No	$I(mA)$	$2Q V$	$Q V$	$1/I A^{-1}$
1	100	15.2	15.2	10.00
2	125	12.0	6.0	8.00
3	175	8.8	4.4	5.71
4	200	7.6	3.8	5.00
5	228	6.6	3.3	4.39

- The slope of $1/I$ versus Q graph for $\nu_0 = 11.25MHz$ is $= 0.636V/A$
- The slope of $1/I$ versus Q graph for $\nu_0 = 13.5MHz$ is $= 0.934V/A$
- The value of g from the slope of graph of $\nu_0 = 11.25MHz$ is $= 1.997$
- The value of g from the slope of graph of $\nu_0 = 13.5MHz$ is $= 2.002$

Experiment 2:ESR - Ravitej Uppu

