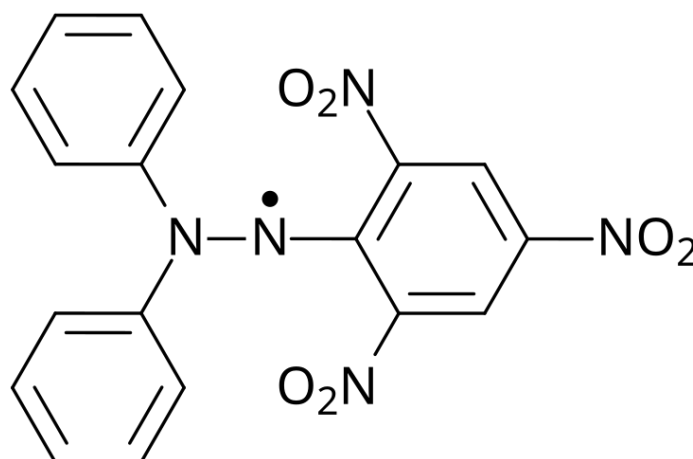


# Experiment 6:

## Electronic Spin Resonance



3rd Year of the Degree in Physics

Experimental Project

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## Contents

<b>1</b>	<b>Introduction</b>	<b>1</b>
<b>2</b>	<b>Experimental Procedure</b>	<b>2</b>
<b>3</b>	<b>Experiment Data and Final Results</b>	<b>2</b>
<b>4</b>	<b>Discussion and Evaluation</b>	<b>4</b>

## Figures Index

### 1 Introduction

In this experiment, we investigate the Electronic Spin Resonance response of the molecule DPPH which is known for having a well-defined resonance signature. By analyzing the resonance frequency as a function of the magnetic field, we aim to determine the Landé factor for the free electron and explore its physical implications in quantum mechanics.

Thus, the objectives of this experiment are:

- To observe the resonance absorption curve of DPPH.
- To determine the resonance frequency as a function of the magnetic field.
- To calculate the Landé g-factor for the free electron and compare it with its theoretical value.

### Theoretical Fundamentals

Electron Spin Resonance (ESR) is a technique used to study systems with unpaired electrons, such as the free radical DPPH. When these electrons are subjected to an external magnetic field, their energy levels split (Zeeman effect), and they can absorb radiation of a specific frequency when the resonance condition is met.

## EXPERIMENT 6. Electronic Spin Resonance

This condition is expressed as:

$$f = g \frac{\mu_B}{h} B$$

where  $\nu$  is the resonance frequency,  $B$  the applied magnetic field,  $\mu_B$  the Bohr magneton, and  $g$  the Landé factor. Experimentally determining this factor allows us to compare the behavior of the electron with the theoretical value for a free electron and gain deeper insight into its quantum dynamics.

## 2 Experimental Procedure

For this experiment, we have used already measured data as the real experiment couldn't be performed because of technical difficulties.

## 3 Experiment Data and Final Results

The measured data is

Frequency (Hz)	U (V)
$37.7051 \times 10^6$	0.5
$40.015 \times 10^6$	0.72
$45.012 \times 10^6$	1.26
$50.06 \times 10^6$	1.7
$55.055 \times 10^6$	2.18
$60.003 \times 10^6$	2.64
$65.009 \times 10^6$	3.04
$70.009 \times 10^6$	3.46

Table 1: Experiment Data  
We have

## Code Explanation

For this experiment, we developed a Python script to compute the magnetic field and Landé  $g$ -factor from the measured data. Below, we explain the main components of the code.

First, we initialize the experimental data as two arrays: the measured resonance frequencies and the corresponding resonance voltages.

## EXPERIMENT 6. Electronic Spin Resonance

```

1 import numpy as np
2 import matplotlib.pyplot as plt
3 import pandas as pd
4
5 f = [37.7051e6, 40.015e6, 45.012e6, 50.06e6, 55.055e6, 60.003e6, 65.009e6, 70.009e6] # Frequen
6 U_r = [0.5, 0.72, 1.26, 1.7, 2.18, 2.64, 3.04, 3.46] # Voltage in V

```

Next, we create empty arrays to store the computed magnetic field values and the corresponding Landé factors. We also define the constants involved in the calculations:

```

1 B = [] # Magnetic field array
2 g = [] # Landé factor array
3 u_B = 9.274e-24 # Bohr magneton in J/T
4 h = 6.62607e-34 # Planck constant in J.s
5 B_o = 3.47e-3 # Conversion factor from volts to teslas (T/V)

```

Using a loop, we calculate the magnetic field and Landé factor for each data point. The magnetic field is computed using:

$$B = B_o \cdot U$$

where  $B_o$  is the conversion factor from volts to teslas. Then we create a DataFrame to visualize the computed values in tabular form:

```

1 for i in range(len(U_r)):
2     B.append(B_o * U_r[i])
3     g.append((h / u_B) * (f[i] / B[i]))
4
5 df = pd.DataFrame({'f (Hz)': f, 'U_r (V)': U_r, 'B (T)': B, 'g': g})
6 print(df)

```

To estimate the Landé factor more accurately, we apply a linear regression based on the resonance frequency equation:

$$f = g \cdot \frac{\mu_B}{h} \cdot B$$

where  $\mu_B$  is the Bohr magneton and  $h$  is Planck's constant. since the function polyfit finds the two parameters of the linear regression, we will keep the one in the first position. This parameter corresponds to the product  $g \cdot \mu_B/h$ . Thus, to isolate  $g$ , we multiply the slope by  $h/\mu_B$ :

```

1 coeff = np.polyfit(B, f, 1)
2 a = coeff[0]*10
3 g_est = a * h / u_B
4 print(f"The estimated Landé factor is {g_est}")

```

## EXPERIMENT 6. Electronic Spin Resonance

Finally, we make the plot of the linear regression.

```

1 f_fit = np.poly1d(coeff)(B)
2
3 plt.plot(B, f, 'o', label='Datos')
4 plt.plot(B, f_fit, '-', label='Ajuste lineal')
5 plt.xlabel('Campo magnético B (T)')
6 plt.ylabel('Frecuencia f (Hz)')
7 plt.title("Frecuencia vs Campo magnético")
8 plt.legend()
9 plt.grid(True)
10 plt.show()

```

## 4 Discussion and Evaluation

**How does the Landé factor relate to the magnetic behavior of a particle in an external magnetic field, and how is it calculated for different systems?**

The Landé factor  $g$  quantifies the proportionality between a particle's magnetic moment and its angular momentum. In the context of electron spin resonance, it describes how an unpaired electron interacts with an external magnetic field. The energy levels split according to the spin states, and this splitting is directly proportional to both the field strength and the Landé factor. For free electrons, the theoretical value is approximately 2.0023. In more complex systems (e.g., atoms or ions with orbital contributions),  $g$  is calculated using:

$$g = \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$

where  $J$ ,  $S$ , and  $L$  are the total, spin, and orbital angular momenta, respectively. This formula accounts for both spin and orbital contributions to the magnetic behavior.

**What is the significance of the Bohr magneton in describing the magnetic behavior of an electron in atoms, and how does it compare to other relevant physical constants in quantum theory?**

The Bohr magneton  $\mu_B$  is the natural unit for expressing the magnetic moment of an electron due to its spin. It plays a central role in quantum magnetism and appears in formulas related to Zeeman splitting and magnetic resonance. Defined as:

$$\mu_B = \frac{e\hbar}{2m_e}$$

## EXPERIMENT 6. Electronic Spin Resonance

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it provides a bridge between macroscopic magnetic behavior and the underlying quantum properties of particles. Compared to other constants in quantum theory (like  $h$ ,  $\hbar$ , or  $e$ ), the Bohr magneton specifically encodes magnetic interactions and is essential in ESR, NMR, and other spin-related phenomena.

### **What are resonant structures? Can you write down two resonant structures of DPPH?**

Resonant structures are different Lewis representations of a molecule that describe the delocalization of electrons within it. These structures do not correspond to distinct isomers but are alternative ways of depicting electron distribution. In molecules like DPPH, resonance helps stabilize the free radical by spreading the unpaired electron across multiple atoms.

Two possible resonance structures of DPPH are:

- One where the unpaired electron is delocalized over the nitrogen atom and adjacent aromatic ring.
- Another where the unpaired electron is shifted toward one of the oxygen atoms in the nitro group.

These structures reflect the conjugated nature of the molecule and explain its stability and strong ESR signal.