Electron Spin Resonance of DPPH

E. K. Dunn*
Department of Physics, University of Kansas, Lawrence, Kansas, USA

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Electron Spin Resonance is very useful in the field of molecular analysis where free electrons are present. It allows insight to the spin interactions of a substance and therefore its structure. The Lande g-factor of DPPH was found by inducing spin flip transitions of a substance via radio wave excitation in a constant magnetic field. The g-factor of DPPH was found to be 1.88±0.08~ in this experiment. Corrections to the apparatus to improve accuracy are outlined.

I. INTRODUCTION

Electron Spin Resonance (ESR) is a special technique used to determine the behavior of semi-free electrons in a paramagnetic material. ESR can be used to calculate the spin interactions of a substance and therefore give clues to the structure. Nuclear Magnetic Resonance –the technique used in MRI machines- is closely related to ESR. MRI machines however, use the magnetic moment of the atoms themselves instead of the lowly electron. Since few stable molecules have free electrons, the existence of those that do in a mixture can be detected by ESR very specifically. This can be especially useful in determining the existence of free radicals in a material.

Electrons have an intrinsic, quantized spin that results in a magnetic moment. When an external magnetic field is applied the magnetic moments of all the electrons align in parallel or antiparallel with the field. The difference in energy of these two states is proportional to the magnetic field and determined by Zeeman splitting. The electrons can be made to flip between the two energy states with the application of resonant electromagnetic radiation of the appropriate energy. A free electron's resonant frequency will be different from a bound electron's. The whole goal of ESR testing is to determine this difference known as the Lande g-factor.

This paper analyzes the almost free electron in α, α, diphenyl-β-pictryl hydrazil also called DPPH for short. A nitrogen pair in the center of the molecule has a trapped electron with no orbital angular momentum. DPPH has been studied extensively with ESR because of its ability to absorb free radicals. A modulated magnetic field and varying driving frequency is used this paper to determine the g-factor of DPPH as compared to the accepted value.[1]

II. DEVICE AND METHODOLOGY

Electrons subject to a magnetic field will split into two energy states given by:

$$U_m = \pm\tfrac{1}{2} g \frac{e\hbar}{2m} B \qquad (1)$$

Where g is the gyromagnetic ratio or Lande g-factor, e is the electron charge, h is Planck's constant, m is the electron mass, and B is the applied magnetic field.[1] Equation 1 can be rewritten replacing $e\hbar/2m$ with μ_B also known as the Bohr Magneton. The application of electromagnetic radiation of the correct energy causes flips between the two states. The energy is given by:

$$\Delta U = h\upsilon_0 = g\mu_B B \qquad (2)$$

Where υ_0 is the frequency of the applied light.[1] Normally the two energy states of electron spin would be equally populated and therefore it would be impossible to detect the change in state. The lower energy state is slightly more populated at room temperature as given by the Boltzmann distribution factor $n(\varepsilon) = Ae^{-\varepsilon}/_{kT}$ and results in net absorbed energy at resonance.

The constant magnetic field is generated with a Helmholtz coil (B) producing approximately 320 μT/A. A secondary set of coils are wound on top of the Helmholtz coil and driven by a resonant RLC circuit. This allows the modulation of the magnetic field producing a field sweep over resonance. The field is modulated by as much as 60% to ease finding resonance. The absorbed energy at resonance is in the form of a reduced Q factor: $Q = \omega L/R$ of the driver coil. With this system the reduced Q factor causes a dip in voltage as the swept magnetic field passes over the resonant value. The input electromagnetic radiation is in the RF range of 30 MHz – 75 MHz with variable frequency and amplitude. For each resonance value the frequency was set and the B field varied. The Earth's magnetic field contributed to the field produced by the Helmholtz coil. This is removed by aligning the Helmholtz coils with the magnetic field of the Earth and taking the average value of the reversed current. The residuals from the two curve fits of magnetic field versus applied RF frequency give the value of Earth's Magnetic field.

III. RESULTS & DISCUSSION

The principle result of this paper is to determine the Lande g-factor of DPPH. The slope of the frequency versus applied magnetic field [Figure 1] was used to calculate the Lande g-factor of DPPH.

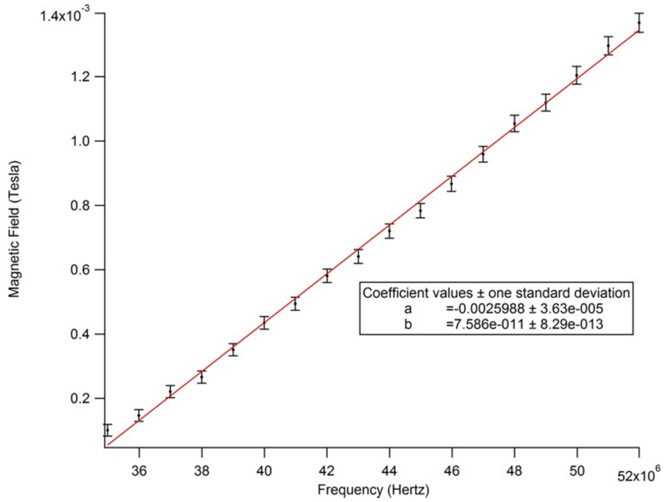

Figure 1: Magnetic Field versus Applied RF Frequency. Slope is used to determine g-factor of DPPH

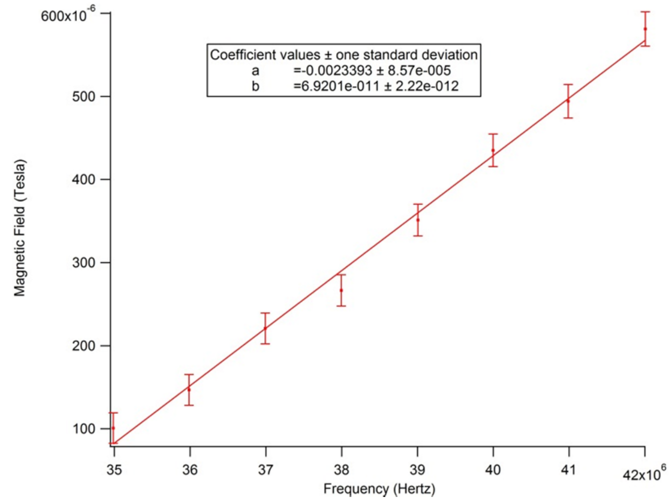

Figure 2: Magnetic Field versus Applied RF Frequency Truncated at f=42 MHz

It was found that $g = 1.88 \pm 0.08$~ and Earth's magnetic field is $B_{EARTH} = 69\,\mu T \pm 11\mu T$. The expected value of the g-factor for DPPH is $g = 2.0036$~.[1] I believe this discrepancy arises from an accidental movement of the apparatus during the experiment. At 42 MHz I accidentally bumped the Helmholtz coil thereby affecting the Earth's magnetic field interaction. This caused the slope to increase and thereby reduced the determined g factor. The data visibly increases in slope after 42 MHz. The g-factor calculated by truncating the data at 42 MHz is $g = 2.1 \pm 0.3$~ which is within experimental uncertainty of the expected value. [Figure 2]

IV. CONCLUSIONS

The Lande g-factor can be useful for determining the structure of a molecule. Though my final value of g differed from the expected, this lab was very insightful. More data should be taken with the Helmholtz coils realigned with the Earth's magnetic field to improve the uncertainty in the g-factor. It is strange to think that such a small change could produce such an easily detectable signal. Electron Spin Resonance is a useful tool to have in any arsenal of molecular analysis.

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[*]Present address: Department of Physics, University of Kansas, Lawrence, KS 66045
[1]"Electron Spin Resonance." Physics Department. University of Kansas.