Trenton Cathcart

03/01/2023

ESR-NMR

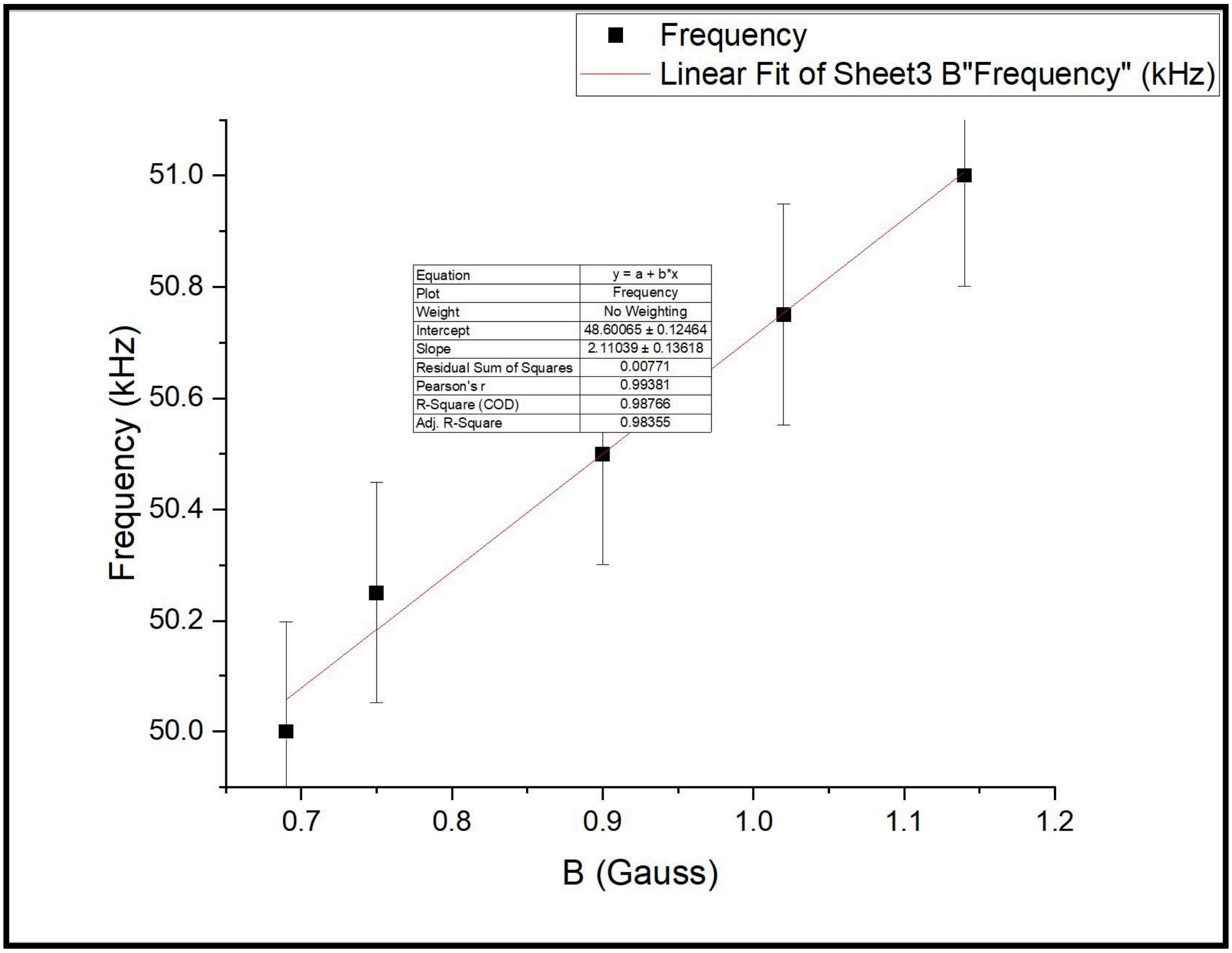

Figure 1. A graph of frequency vs magnetic field measured from the DPPH salt using the ESR set up

Q1. What is the value of the g-factor determined from the experiment for DPPH? What is the estimated error in the g-factor for DPPH?

To calculate the g-factor for the DPPH sample, you can use the following formula: $g_s = \frac{\hbar \cdot \Delta v}{\mu_B \cdot \Delta B}$

where:

- g_s is the g-factor for the DPPH Sample
- ħ is the Planck's constant $(1.05457 \times 10^{-34}\, Js)$
- Δv is the difference in frequency (in Hz)
- μ_B is the Bohr magneton $(9.274 \times 10^{-24}\, \frac{J}{T})$
- ΔB is the difference in magnetic field (in Tesla)

Trenton Cathcart
03/01/2023

From the linear fit plot shown above within **Figure 1**, you have the slope (b) = 2.11039 ± 0.13618$\frac{KHz}{Gauss}$, which represents the relationship between the frequency (v) and the magnetic field (B). This slope can be used to find $\frac{\Delta v}{\Delta B}$.

$$\frac{\Delta v}{\Delta B} = 2.11039\ \frac{kHz}{Gauss}$$

To convert the slope to Hz/Tesla, you need to apply the following conversions:

- 1 kHz = 1000 Hz
- 1 Gauss = 0.0001 Tesla

$$\frac{\Delta v}{\Delta B} = 2110.39\frac{Hz}{Gauss} \times \frac{10{,}000\ Gauss}{1\ Tesla} = 21103900\ \frac{Hz}{Tesla}$$

Now, you can plug this into the g-factor formula:

$$g_s = \frac{1.05457\times10^{-34}\ Js \times 21103900\ \frac{Hz}{Tesla}}{9.274\times10^{-24}\ \frac{J}{T}} = 2.399$$

g-factor ≈ 2.399

So, the g-factor determined from the experiment for the DPPH sample is approximately 2.399. Keep in mind that there is an estimated error in the slope (±0.13618).

Now for calculating the slope error:

$$\text{Slope error: } \frac{\Delta v}{\Delta B} = 0.13618\frac{Hz}{Gauss} \times \frac{10{,}000\ Gauss}{1\ Tesla} = 1361.8\frac{Hz}{Tesla}$$

$$\text{Error } g_s = \frac{1.05457\times10^{-34}\ Js \times 1361.8\frac{Hz}{Tesla}}{9.274\times10^{-24}\ \frac{J}{T}} = 0.015$$

Also from a quick google search it can be seen that the actual G factor of DPPH is 2.003621, Therefore our value is largely incorrect due to error from the machine, even with the estimated error amount

Trenton Cathcart
03/01/2023

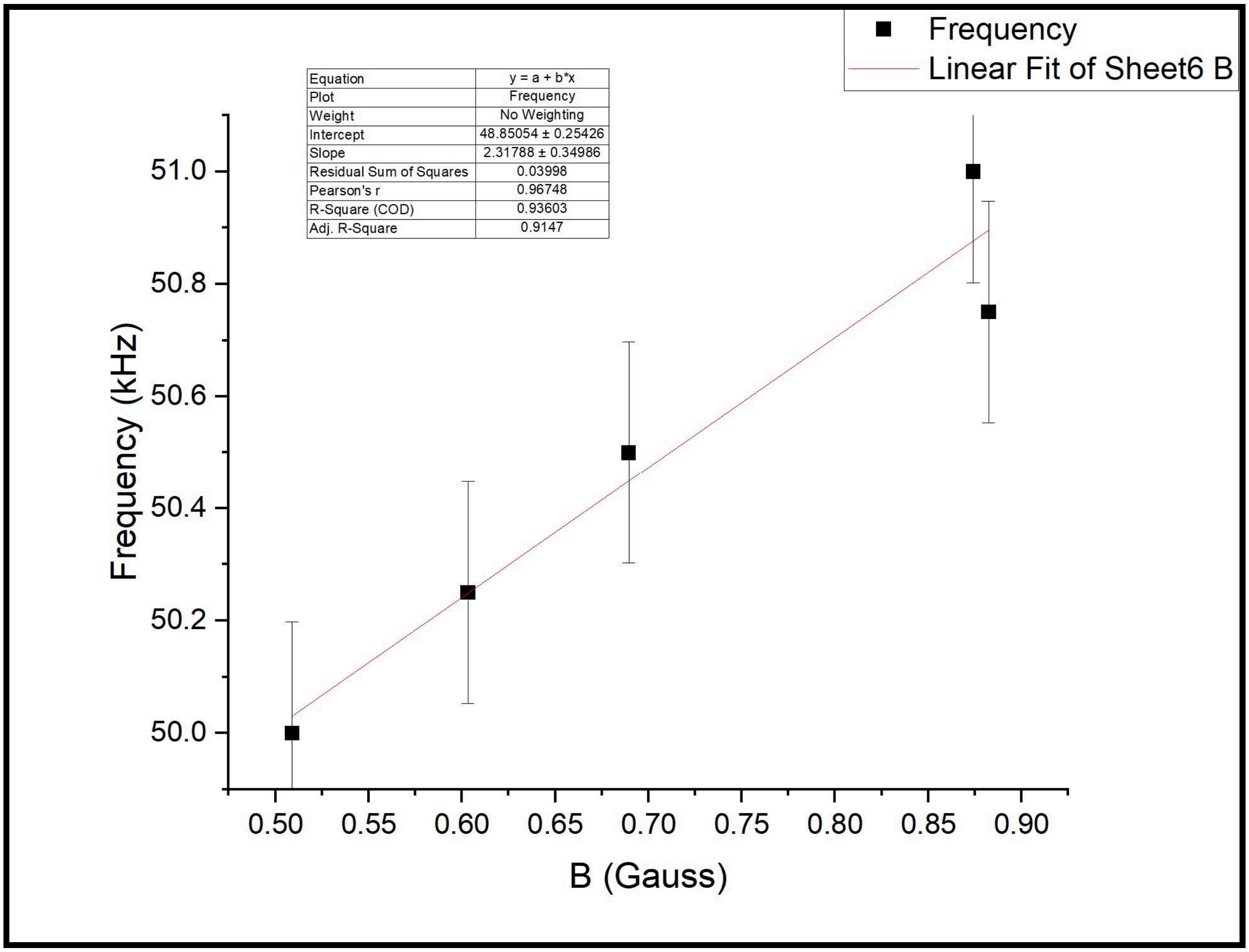

Figure 2. A graph of frequency vs magnetic field measured from the TNCQ using the ESR set up

Q1. What is the value of the g-factor determined from the experiment for TCNQ? What is the estimated error in the g-factor for TCNQ?

To calculate the g-factor for the DPPH sample, you can use the following formula: $g_s = \frac{\hbar \cdot \Delta v}{\mu_B \cdot \Delta B}$

where:

- g_s is the g-factor for the DPPH Sample
- ħ is the Planck's constant $(1.05457 \times 10^{-34} Js)$
- Δv is the difference in frequency (in Hz)
- μ_B is the Bohr magneton $(9.274 \times 10^{-24} \frac{J}{T})$
- ΔB is the difference in magnetic field (in Tesla)

From the linear fit plot shown above within **Figure 2**, you have the slope (b) = 2.31788 ± 0.34986$\frac{KHz}{Gauss}$, which represents the relationship between the frequency (v) and the magnetic field (B). This slope can be used to find $\frac{\Delta v}{\Delta B}$.

$$\frac{\Delta v}{\Delta B} = 2.31788\ \frac{kHz}{Gauss}$$

To convert the slope to Hz/Tesla, you need to apply the following conversions:

- 1 kHz = 1000 Hz
- 1 Gauss = 0.0001 Tesla

$$\frac{\Delta v}{\Delta B} = 2.31788\frac{Hz}{Gauss} \times \frac{10{,}000\ Gauss}{1\ Tesla} = 23178800\ \frac{Hz}{Tesla}$$

Now, you can plug this into the g-factor formula:

$$g_s = \frac{1.05457\times10^{-34}\ Js \times 23178800\ \frac{Hz}{Tesla}}{9.274\times10^{-24}\ \frac{J}{T}} = 2.636$$

g-factor ≈ 2.636

So, the g-factor determined from the experiment for the TCNQ sample is approximately 2.636. Keep in mind that there is an estimated error in the slope (±0.34986).

Now for calculating the slope error:

$$\text{Slope error: } \frac{\Delta v}{\Delta B} = 0.34986\frac{Hz}{Gauss} \times \frac{10{,}000\ Gauss}{1\ Tesla} = 3498.6\frac{Hz}{Tesla}$$

$$\text{Error } g_s = \frac{1.05457\times10^{-34}\ Js \times 3498.6\frac{Hz}{Tesla}}{9.274\times10^{-24}\ \frac{J}{T}} = 0.397$$

Q2. Briefly describe the fundamental interaction between the E-M microwave radiation and the free-radical spin that enables the observation of the ESR effect.

A. To answer this question, I need to explain the fundamental interaction between electromagnetic (E-M) microwave radiation and the free-radical spin that enables the observation of the electron spin resonance (ESR) effect. No additional data is required. ESR, also known as electron paramagnetic resonance (EPR), is a spectroscopic technique that observes the interaction between unpaired electron spins and an external magnetic field. Free radicals are molecules or atoms with unpaired electrons in their outermost shell. When a sample containing free radicals is placed in a magnetic field, the unpaired electron spins align themselves either parallel or antiparallel to the magnetic field direction. These two spin states have different energy levels. The energy difference between these two spin states is proportional to the strength of the magnetic field. When the sample is exposed to E-M microwave radiation, the radiation frequency is tuned to match the energy difference between the two spin states. If the radiation frequency matches this energy difference, the unpaired electrons can absorb the energy from the microwave radiation and undergo a transition from the lower energy state to the higher energy state. This absorption of energy is the basis of the ESR effect. In summary, the fundamental interaction between E-M microwave radiation and free-radical spin that enables the observation of the ESR effect is the absorption of microwave radiation energy by unpaired electrons, causing a transition between two spin states with different energy levels when the radiation frequency matches the energy difference between these states.

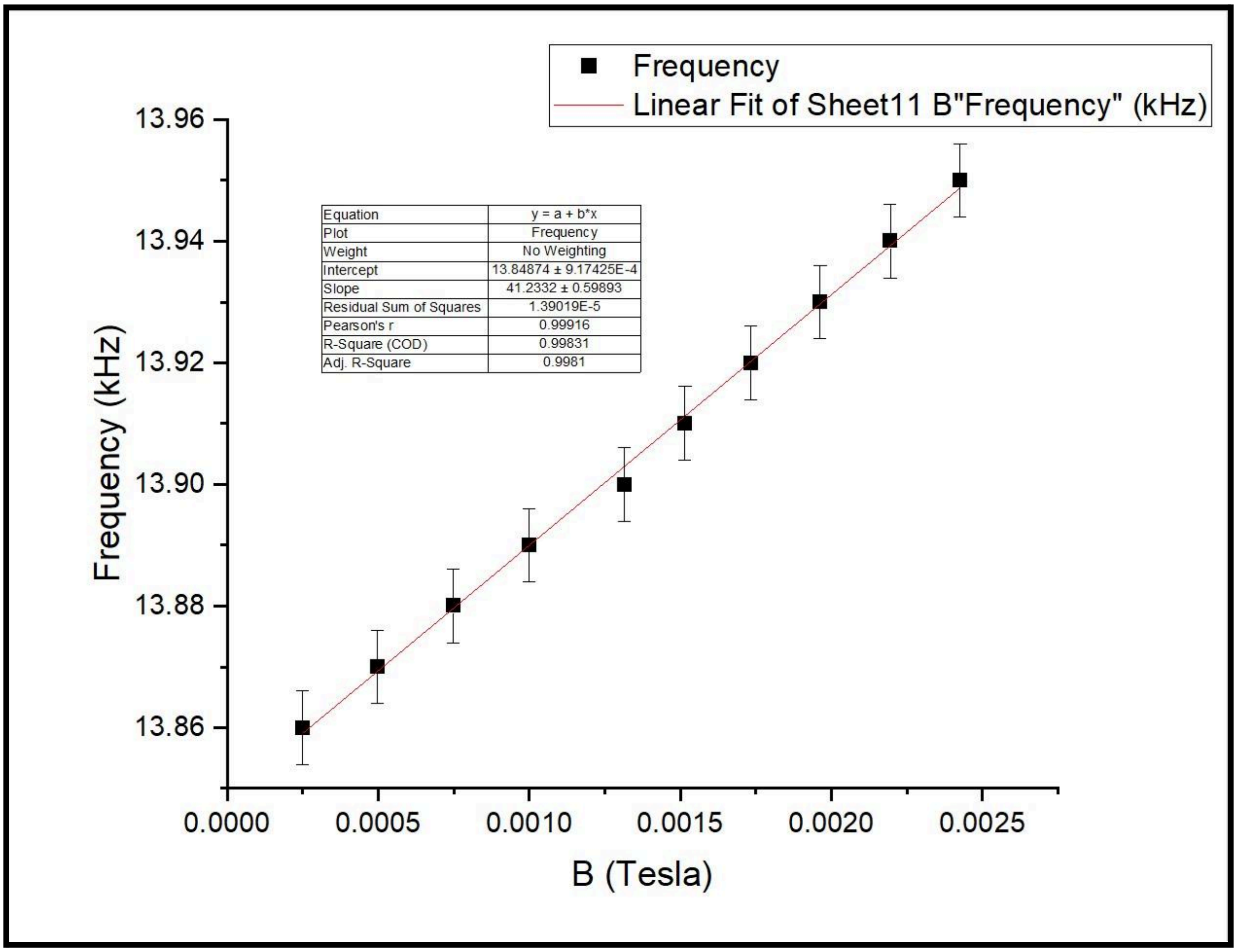

Figure 3. A graph of frequency vs magnetic field measured from the HBrF using the NMR set up

Q3. What is the value of the γ-factor determined from the experiment for the HBrF sample? What is the estimated error in the γ-factor value?

Given the slope(b) from the above **Figure 3.** slope(b) = 41.2332 $\frac{kHz}{Gauss}$, we will first convert it to $\frac{Hz}{Gauss}$:

Slope = 41.2332 $\frac{kHz}{Gauss}$ * 1000 $\frac{Hz}{Gauss}$ = 41233.2 $\frac{Hz}{Gauss}$

Trenton Cathcart
03/01/2023

Now, we'll apply the tip formula to calculate the experimental γ value:

$\gamma = 2\pi \times (slope) \times 0.1$
$\gamma = 2\pi \times (41233.2 \frac{Hz}{Gauss}) \times 0.1$
$\gamma \approx 25902.4 \frac{rad}{s \cdot T}$
Next, let's calculate the error in the experimental γ value:

Error in slope = 0.59893 $\frac{kHz}{Gauss}$ * 1000 $\frac{Hz}{Gauss}$ = 598.93 $\frac{Hz}{Gauss}$
Error in $\gamma = 2\pi \times (Error\ in\ gamma) \times 0.1$
Error in $\gamma = 2\pi \times (598.93 \frac{Hz}{Gauss}) \times 0.1$
Error in $\gamma = 376.2 \frac{rad}{s \cdot T}$

So, the experimental magnetogyric ratio (γ) for the HBrF sample is approximately $25902.4 \pm 376.2 \frac{rad}{s \cdot T}$.

Q4. Briefly describe the fundamental interaction between the E-M microwave radiation and the nuclear spin that enables the observation of the NMR effect.

A. Nuclear Magnetic Resonance (NMR) is a phenomenon that arises from the interaction between nuclear spins and an external magnetic field. The fundamental interaction in NMR involves the absorption and emission of electromagnetic (E-M) microwave radiation by atomic nuclei with nonzero nuclear spins when they are exposed to a magnetic field. When an external magnetic field is applied, the nuclear spins align themselves either parallel or antiparallel to the field. This creates discrete energy levels that depend on the strength of the applied magnetic field and the magnetogyric ratio (γ) of the specific nucleus. The energy difference between these levels is proportional to the strength of the applied magnetic field. The E-M microwave radiation provides the energy required for the transition between these energy levels. When the energy of the radiation matches the energy difference between the spin states, the nuclei absorb the radiation and undergo a transition from lower to higher energy state, which is called resonance. This transition results in a change in the magnetic moment of the nuclei, creating a detectable signal. The NMR effect is observed when the nuclei return to their equilibrium state, either by transferring the energy to their surroundings or by emitting radiation. The emitted radiation is detected and processed, providing valuable information about the chemical environment and the structure of the molecules in which the nuclei reside. In summary, NMR is based on the interaction between nuclear spins and an external magnetic field, and the absorption and emission of E-M microwave radiation. This interaction leads to the observation of the NMR effect, which provides insights into the structure and properties of molecules.