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# ELECTRON SPIN RESONANCE

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## ABSTRACT

Electron Paramagnetic Resonance (EPR) or Electron Spin Resonance (ESR) is employed to study systems with unpaired electrons, such as free radicals and transition metal ions. EPR provides valuable information about the structure and interactions of paramagnetic species within the system. In this study, EPR spectra of DPPH and MnCl2/H2O were analyzed to determine the paramagnetic species present. The g-factor, calculated as 0.71449 v(GHz)/B(kG), plays a crucial role in characterizing the samples. The investigation revealed multiple EPR peaks in MnCl2/H2O, suggesting the presence of diverse paramagnetic centers. However, the calculated average g value deviated significantly from the expected value, indicating a potential miscalculation of magnetic field values during the sweep range analysis. To ensure accuracy, the researchers recommended reevaluating the calculations and methodology. These findings contribute to a deeper understanding of paramagnetism and its potential applications in various scientific fields. Further research into MnCl2/H2O's properties holds promising prospects for un-king new insights into paramagnetic phenomena.

**Keywords:** g-factor, peaks, electrons, free radicals, paramagnetic

## I. INTRODUCTION

Electron Paramagnetic Resonance (EPR), commonly referred to as Electron Spin Resonance (ESR), analyzes systems containing unpaired electrons, such as free radicals and transition metal ions. EPR provides information with respect to the structure of the system in which the unpaired electrons are found, including the identity, oxidation, spin state, and the interactions of paramagnetic ions within the lattice of the system. The g-factor, with a value of 0.71449 v(GHz)/B(kG), is a ratio of the frequency received from the EPR spectrometer and the magnetic field at the point where the tangent line crosses the signal baseline (Figure 1). It is worth noting that free electrons If each electron occupies a different energy level, shown in Figure 2, a “high-spin” state is observed, with a net spin of S = 1/2. If each electron were to pair up in low-energy states, we would observe a “low-spin” state. It is possible to observe changes in spin states in the event that ligands are interacting with one another. A zero-field split case can also be observed in areas with local magnetic fields thanks to other atoms in the lattice, which remove the degeneracy of the S-state (EPR handout). In this experiment, we analyzed the EPR spectra of DPPH and MnCl2/H2O in order to scientifically determine the paramagnetic species. An in-depth analysis of the samples was performed using parameters such as microwave frequency, power, center field, sweep range, modulation field and frequency, scan time, g-value, and temperature. We used electrochemical titrations and an anaerobic cell to assist the preparation of our samples, as well as the Bruker ER 200D X-band spectrometer and a Q-band spectrometer in order to perform the experiment itself.

## II. METHODOLOGY

In our comprehensive analysis of the DPPH and MnCl2/H2O samples, we meticulously set specific instrumental parameters to ensure the acquisition of reliable and qualifying results during the experimental process. These parameters played a critical role in shaping the outcome of our investigations and included the following key factors: Microwave Frequency, Microwave Power, Center Field, Sweep Range, Modulation Field, Modulation Frequency, Scan Time, Gain, and Temperature.

**Microwave Frequency-** The microwave frequency served as a fundamental parameter to determine the frequency of electromagnetic radiation applied during the electron paramagnetic resonance (EPR) spectroscopy measurements. Controlling the microwave power allowed the achievement of optimal signal-to-noise ratios while avoiding damage due to excess power levels.

**Center Field-** The center field variable was set to 3 kg (equivalent to 3000 G) for our MnCl2/H2O sample. It played a pivotal role in determining the central magnetic field position around which the EPR spectra were measured. Additionally, the Sweep Range determined the extent of the magnetic field variation during the EPR experiment, allowing us to probe spectral features of interest effectively.

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**Modulation Field and Modulation Frequency**

These parameters were critical and were utilized to implement the modulation of the magnetic field during EPR spectroscopy. This modulation enhanced the signal-to-noise ratio and facilitated the detection of weak spectral features, providing valuable insights into the electronic properties of the samples.

**Scan Time**

The scan time defined the duration of data collection at each field point during the EPR measurements. By optimizing the scan time, we balanced the trade-off between spectral resolution and acquisition speed, ensuring high-quality data while minimizing experimental time.

**Gain**

This was a sensitivity parameter that amplified the detected signals appropriately. Careful calibration of this parameter allowed us to optimize the signal levels, leading to accurate and reproducible measurements.

**Temperature**

The temperature was precisely maintained during the experiments to ensure sample stability and reproducibility. The thermal stability of the samples significantly impacted the observed spectral features and allowed us to gain insights into temperature-dependent properties.

The results of this experiment will be displayed in section 3. For the DPPH sample in Figure 1, we focused on determining the field positions of the peaks and subsequently calculated the separation between the two peaks using the EPR resonance condition.

For the MnCl2/H2O sample, a comparative approach was undertaken, where we analyzed the error between the experimental and expected values. This involved meticulous examination of the EPR spectra and identifying any major discrepancies between the two sets of data.

## III. MODELING AND ANALYSIS

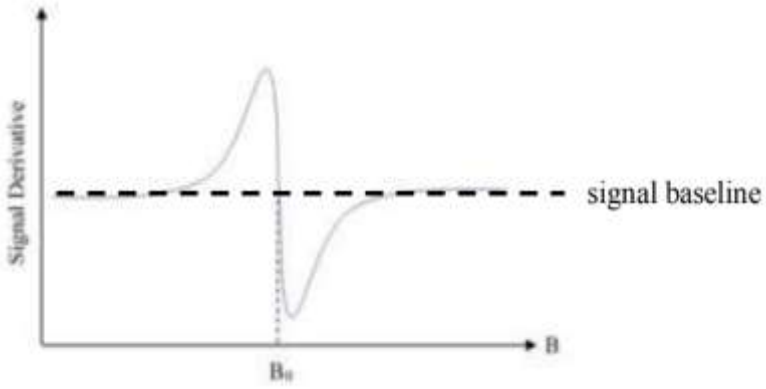


**Figure 1:** Field positions of the peaks

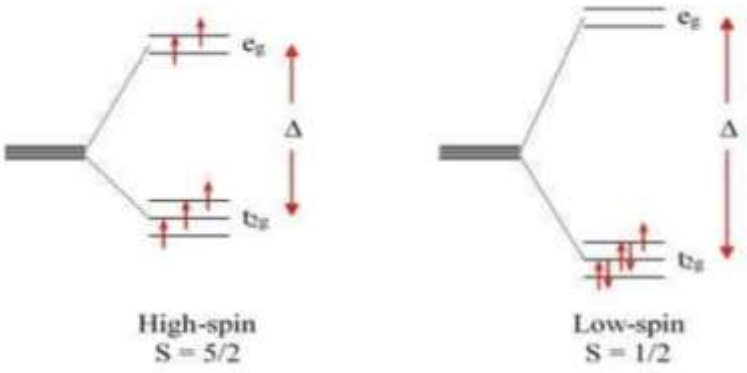


**Figure 2:** High spin resonance vs low spin resonance

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## IV. RESULTS AND DISCUSSION

In our DPPH study, we utilized specific parameters to determine the properties of the paramagnetic species present. One of the key parameters we used in these experiments is the magnetic field strength, commonly represented as the center field (B0) value. In this case, the calculated center field value was recorded as 3.2 kG, which is equivalent to 3200 G. We also calculated the Bi and Bf values are 2950 G and 3450 G, respectively. These values represented the positions at which EPR peaks occurred. The Bi value corresponds to the position for the negative peak, while the Bf value correlates with the position for the positive peak. To analyze the experimental g-factor, we used the resonance condition formula, using Planck's constant (h), microwave frequency (v), and the Bohr magnetron. This value came out to be approximately 2.0085 GHz/kG.

In our study of MnCl2/H2O, we were provided with key parameters: the center field (Bo) value of 3 kG, or 3000 G, and the initial Bi and final Bf values of 500 G and 5,500 G, respectively. An analysis of these values led us to a calculation of the intermediate B values: B1 = 925 G, B2 = 1340 G, B3 = 1744 G, B4 = 2170 G, B5 = 2585 G, and B6 = 3000 G.

During our investigation, we also measured the corresponding g values at each B point: 7.06 GHz/kG at B1, 4.876 GHz/kG at B2, 3.723 GHz/kG at B3, 3.011 GHz/kG at B4, 2.527 GHz/kG at B5, and 2.178 GHz/kG at B6. Upon calculating the average g value, we obtained 3.895 GHz/kG, which significantly deviates from our expected G0 value of 2.178 GHz/kG.

The discrepancy in the average g value could be attributed to a potential miscalculation of our B0 or any of the varying B values during the sweep range analysis. It's possible that an error occurred in identifying or computing the crucial B0 value, leading to discrepancies in the subsequent B values.

To ensure the accuracy of our findings, it may be prudent to reevaluate the calculations and double-check all the steps involved in determining the B0 and other B values. Additionally, a thorough review of the methodology used for the sweep range analysis is essential to identify any potential sources of error. By meticulously scrutinizing our procedures, we can enhance the reliability of our results and draw more accurate conclusions about the MnCl2/H2O system.

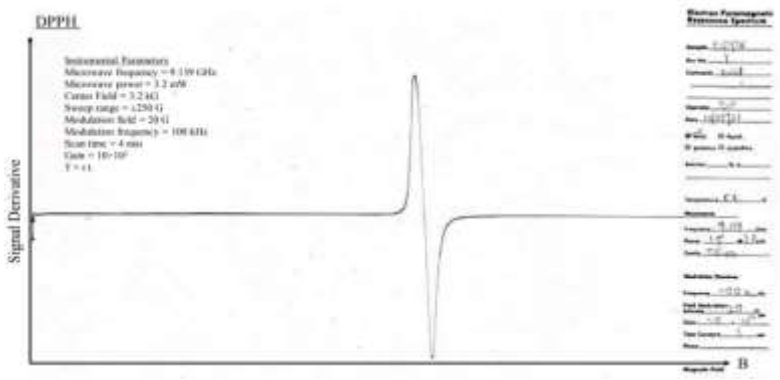


**Figure 3:** DPPH EPR graph

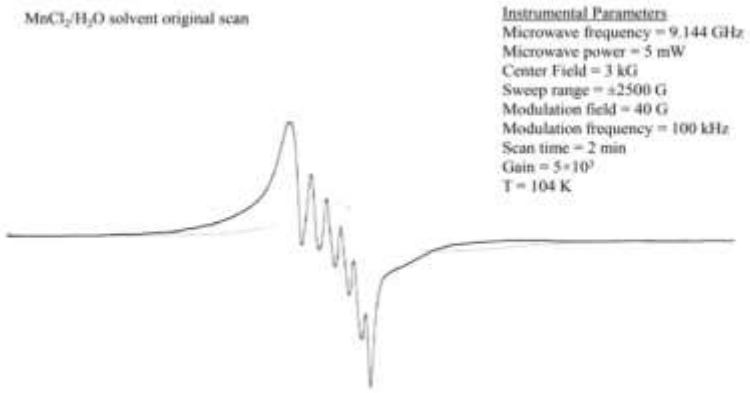


**Figure 4:** MnCl2/H2O EPR graph

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## V. CONCLUSION

The investigation of MnCl2/H2O using EPR spectroscopy revealed multiple EPR peaks (B1 to B6), indicating the presence of distinct paramagnetic species or molecular environments within the sample. The variations in g values at different magnetic field positions provided valuable insights into the electronic structures and interactions of these paramagnetic constituents. These findings offer a comprehensive understanding of MnCl2/H2O's paramagnetic properties, potentially leading to applications in catalysis, material science, and biological research.

These results contribute significantly to the broader knowledge of paramagnetism and its relevance in various scientific disciplines. As the investigation continues, MnCl2/H2O promises to remain an intriguing subject of study, driving further exploration into the captivating world of paramagnetic phenomena.

## VI. REFERENCES

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