Temperature-dependent Electron Paramagnetic Resonance (EPR) of the organic radical dithiazolyl-p-naphthoquinone-1,3 (DTANQ) was investigated. Analysis produced the energy gap between the singlet and triplet spin states of the unpaired electrons interacting within the compound. This energy difference is proportional to the exchange constant J which corresponds to the strength of the exchange interaction between these electrons, and therefore provides information on the magnetic properties of the compound.

**DTANQ RADICAL**

Organic radicals form an excellent model system for studying magnetic interactions as their properties can be tuned with chemical substitution. In the solid-state, DTANQ radicals form dimers with an effective spin of S=1/2 in each molecule.

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**Theory**

In a system with two interacting spin-1/2 particles, the two spins can have four possible orientations: ↑↑, ↑↓, ↓↑, ↓↓, where ↑↓ spins are represented by up/down arrows. The two ↑↓ basis states are indistinguishable and are therefore represented by two possible combinations of each other.

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To minimize the total energy of the system, the energy of the states given by these orientations are split, giving rise to a gap (Δ) in the presence of antiferromagnetic interaction, the energy of the singlet state is lower in energy compared to the degenerate triplet states.

The degeneracy of triplet states is lifted by magnetic field, and transition across the triplet states (shown by red arrows in Figure 4) can be observed by EPR spectroscopy.

**RESULTS AND DISCUSSION**

Absorption increases with increasing temperature up to 150 K. Above 150 K, a decreasing intensity with increasing temperature is observed.

Intensity of the EPR signal given by the isolated dimer model (IT) is related to the probability of electrons existing in the triplet states derived from the Boltzmann distribution function:

\[
I(T) = \frac{2N(0) e^{\Delta E / kT}}{1 + e^{\Delta E / kT}}
\]

\[
\Delta = \sqrt{\frac{4J^2}{3kT}}
\]

Figure 5 shows hardly any contribution from the triplet state transitions (side broad peaks) at 5 K. Their contribution increases with temperature, as there is increasing thermal excitation of electrons from the singlet into the triplet states.

**CONCLUSION**

X-band EPR is used to study the exchange interaction in DTANQ dimers. The antiferromagnetic coupling between the molecules in the dimers is verified by the spectra. The temperature-dependent study provides an approximate estimate of J ≈ 380 K using the isolated dimer model. However, in order to obtain more quantitative information, the dependency of J on temperature and inter-dimer interactions must be taken into account.

**REFERENCES AND ACKNOWLEDGMENTS**

[1] [University of West Florida, Pensacola, FL, USA]

[2] [University of Guelph, Guelph, Ontario, CA]

**ABSTRACT**

Organic radicals form an excellent model system for studying magnetic interactions as their properties can be tuned with chemical substitution. In the solid-state, DTANQ radicals form dimers with an effective spin of S=1/2 in each molecule.

**ELECTRON PARMAGNETIC RESONANCE**

Electron paramagnetic resonance (EPR) spectroscopy is a noninvasive technique that yields important information such as structural and electronic properties on a chemical system containing unpaired electrons. EPR relies on the Zeeman Effect (illustrated in Figure 4) in which the degenerate energy levels are split in the presence of an external magnetic field. A spectrum is obtained when electrons transition between split energy levels by absorbing incoming radiation. The signal therefore corresponds to the energy difference between these levels. Fundamental equation for EPR:

\[
E = h\nu = g\mu_B B
\]

where h is Planck’s constant, \(\nu\) is frequency of incoming radiation, g is gyromagnetic ratio, \(\mu_B\) is Bohr’s magnetron, and B is magnetic field strength.

**Instrument**

• Spectrometer: Bruker Elexsys E 580
• Frequency: X-band (= 9.6-9.8 GHz)

**Experimental Parameters**

• Magnetic Field: 3000-3800 G
• Temperature: 5-300 K