Experiments where carried out to gain understanding about high-frequency/field EPR (HF-EPR) and its applications in studying magnetic materials. In this experiment powder EPR data were collected on a high-symmetry (3-fold symmetry) mononuclear Ni(II) complex to study its electronic structure. The data were analyzed employing two unique methods, each using the same energy Hamiltonian and parameter set.

Introduction

EPR (Electron Paramagnetic Resonance) spectroscopy is employed to study elements/compounds that possesses unpaired electrons. When an electron is excited in the presence of an external magnetic field it will process about that magnetic field at a frequency called the Larmor Frequency.

The spins can align either parallel or antiparallel to the external magnetic field creating an energy gap known as the Zeeman effect. As the magnetic field is swept, the Larmor frequency increases, and when the Larmor frequency is equal to the energy of the applied microwave frequency, the electrons can absorb the microwave energy and move to a higher energy state. The energy is then given back when the electron relaxes back to its initial state. This excitation gap is the origin of the EPR experiment. Furthermore, the electrons in some systems exhibit a preferred directional orientation in the absence of an external magnetic field. This splits the energy levels and thus the system becomes magnetically anisotropic. EPR is an exceptionally good tool for studying the electronic structure and anisotropy of magnetic materials.

The high-frequency/field EPR data were collected at the National High Magnetic Field Laboratory (NHMFL) Electron Magnetic Resonance (EMR) facility using a transmission probe in which microwaves are propagated through cylindrical light-tight plastic. High-frequency microwaves were generated by a phase-locked Vistadant solid-state source operating at 91.5 GHz, followed by a chain of multipliers and amplifiers. High magnetic fields were provided by a 17 T superconducting magnet.

Experiment

201.6 GHz @ 2.5K

Discussion

Because the total spin (S) is small (S = 1/2), it is enough sufficient to describe the high symmetry (C3v) only two terms are required in the Hamiltonian to describe the system, and only two adjustable parameters, g and D. The first term \( \mathbf{\mu} \mathbf{B} \mathbf{g} \cdot \mathbf{S} \), where \( \mathbf{\mu} \mathbf{B} \) is the Bohr magneton, \( \mathbf{B} \) is the applied magnetic field, \( \mathbf{g} \) is the Landé g-factor and \( \mathbf{S} \) is the spin-operator describes the Zeeman energy, as discussed in the introduction.

while the second term \( DS \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \down arrow

The data was analyzed employing two unique methods, each using the same energy Hamiltonian and parameter set.