# Locating the Hard Plane of $Fe_8$ using a 9/5/1 Superconducting Vector Magnet

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## Overview

$Fe_8$ ($[Fe_8O_2(OH)_{12}(tacn)_6]Br_8(H_2O)_9$, Figure 1) is a biaxial single molecule magnet that has been studied extensively due to its interesting magnetic properties. The magnetic properties arise from 8 exchanged coupled $Fe^{III}$ ions, where 6 spin-up ions antiferromagnetically couple to 2 spin-down ions, yielding a total spin value of $S$ = 10. The easy axis of the molecule is defined as the preferred magnetization orientation. The hard plane of the molecule is the plane perpendicular to the easy axis. The magnetic anisotropy parameters, $D$ = -0.205 cm$^{-1}$ and $E$ = 0.038 cm$^{-1}$ (Barra, A. L., D. Gatteschi, et al. (2005)), have been measured with various techniques, including high field electron paramagnetic resonance, inelastic neutron scattering, and far-infrared spectroscopy. In this study, we aim to show how a 3D vector magnet can be used to locate the hard plane of $Fe_8$ and potentially provide more information on this molecule.

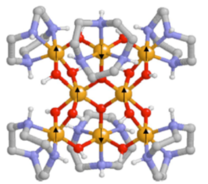


*Figure 1: The structure of $Fe_8$ is presented here with $Fe^{III}$ atoms represented by the orange spheres (red: oxygen, purple: nitrogen, gray: carbon). $Fe_8$ is a biaxial molecule with a spin value of S=10. (Letard, I., P. Sainctavit, et al. (2007))*

## Instrumentation

The instrument used in this study is a 9/5/1 superconducting vector magnet (Cryogenic Ltd.) that consists of 3 magnets arranged orthogonally. The X direction consists of a 5T inner split-coil magnet; the Y direction consists of a 1T outer split-coil magnet; and the Z direction consists of a 9T solenoid base magnet. A picture of the vector magnet can be seen in figure 2 with the XYZ coordinate axes labeled. The presence of the three magnets allows us to study the magnetic properties of samples in different orientations with a rotating field only. The coils and the placement of the probe were calibrated using DPPH, which is commonly used to calibrate the field in EPR experiments. Our calibrations improved the factory calibrations, which were done by calculating the field to current ratio based on the size of the magnets.

| | |
|---|---|
| 15 | Nitrogen Reservoir |
| 16 | 40K Shield |
| 17 | Helium Reservoir |
| 18 | 1T Split-Pair (Y) |
| 19 | 9T Solenoid (Z) |
| 20 | 5T Split-Pair (X) |

*Table 1 (above): Labels for vector magnet drawings*

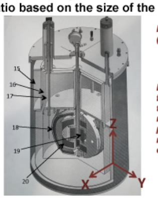
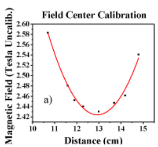


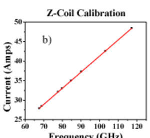

*Figure 2 (left): 3D image of vector magnet. (Cryogenic Ltd.)*

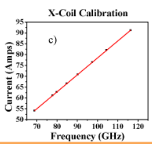
*Figure 3 (below): Calibration curves used for finding the field center (a) and checking the Z (b), X (c), and Y (d) coils of the vector magnet. Y-coil calibration was done in the presence of the X-coil due to the resonance field of DPPH being out of range of the Y-coil.*

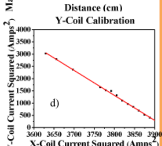
*Table 2 (below): The field to current ratios for each coil that were calibrated by the EPR signal from DPPH.*

| | Z-Coil | X-Coil | Y-Coil |
|---|---|---|---|
| Our Calibrated Field to Current Ratio | 862.80 G/A | 456.11 G/A | 142.40 G/A |



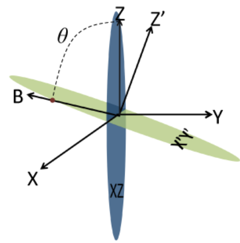




## Methods

A single crystal was placed in a random orientation on the endplate of a vertical cavity. 360° XZ plane sweeps were done at a constant field (B) as the probe was rotated by 15° steps counterclockwise to a new position after every sweep.

*Figure 4: The blue plane and XYZ coordinate axis correspond to the frame of reference of the magnet. The green plane and X'Y'Z' coordinate axis correspond to the frame of reference of the hard plane (X'Y' plane) and easy axis (Z') of $Fe_8$. θ represents the angle of the magnetic field in the XZ plane; the red dot denotes the intersection between the hard plane and field rotation plane. The probe was rotated around the Z axis.*




## Experimental Data

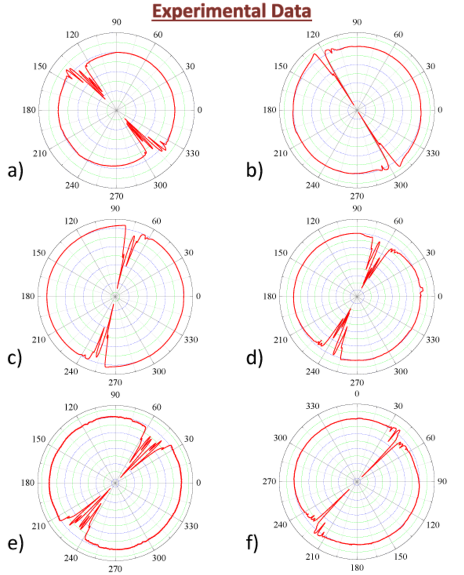
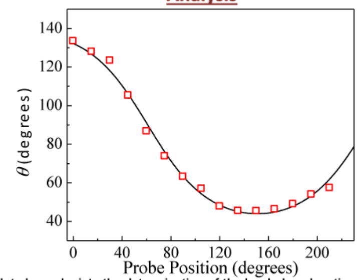


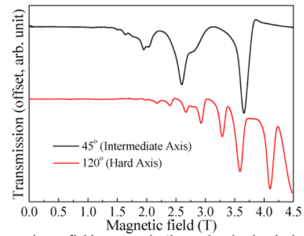

*Figure 5: Representative angle swept EPR spectra in the magnet's XZ plane obtained at T=2K, f=51.5GHz, and 3.5 tesla. The cavity transmission signal is recorded as a function of the field orientation. The different spectra correspond to the position of the probe: a)0°, b)30°, c)60°, d)90°, e)120°, f)150°. Variations in the spectra occur due to the field intersecting with the hard plane at different orientations and the presence of transverse anisotropy. The dips in the spectra correspond to the EPR transitions when the field is located close to the molecular hard plane.*

## Analysis




The plot above depicts the determination of the hard plane location as a function of the probe position and $\theta$. The open red squares represent the intersection of the magnetic field and hard plane obtained from experiments. The easy axis orientation of the molecule was found by searching the direction which is perpendicular to the experimentally determined hard plane. The best fit showed that the easy axis is 46° away from the magnet's Z axis. The black curve represents the simulation of the hard plane orientation based on the easy axis direction of the molecule.

## Field Sweeps in Molecular Hard Plane




The figure above shows field sweeps in the molecular hard plane at different probe positions (45° and 120°). The data were collected with the field applied close to the molecular intermediate axis (45°) and hard axis (120°), and reveals that the Fe8 system exhibits significant transverse anisotropy.

## Conclusion

The results of this experiment demonstrate the ability of a 3D vector magnet to locate the hard plane of single molecule magnets from single crystal samples. With this knowledge, proper orientation of the sample can be made to gather further information about the magnetization properties of the sample. In a biaxial system, such $Fe_8$, the location of the hard and intermediate axes can be found through angle sweeps and are further confirmed with field sweeps.

## References and Acknowledgements

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