MAGNETIZATION AND ELECTRON PARAMAGNETIC RESONANCE OF RARE EARTH BASED MOLECULAR MAGNETS

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Single-molecule magnets (SMMs) provide a rare opportunity for both quantum phenomena and basic magnetism to be studied on a macroscopic scale. Due to their unique properties, they also have potential applications in both quantum computation and high density data storage. Recently, 4f-3d heterometallic complexes have been shown to be capable of producing single molecule magnet behavior. Unlike the well understood 3d metal SMMs, the mechanism for producing this property in 4f-3d compounds has yet to be fully understood. Here, we have analyzed four novel compounds of such structure: DyV, TbPdTb, Tb2Ni2, and Tb4Cu. Using a pulsed magnetic field up to 20 T at temperatures of 4.2 K and below, magnetization curves and electron paramagnetic resonance (EPR) spectra were obtained. The magnetic spin states and the Landé g-factor of the samples were determined. Resonances found in the EPR spectra were attributed to certain spin states of the molecules, which was then used to determine the magnetic state of the materials, as well as the presence of spin coupling. The total angular momentum of the component magnetic moments was determined by plotting the Brillouin function against the magnetization curves. Time dependent magnetization curves will be determined for two of the samples which had shown slight hysteresis. This should show further insight into the magnetic structure of the samples.

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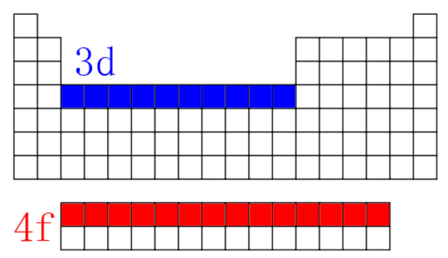
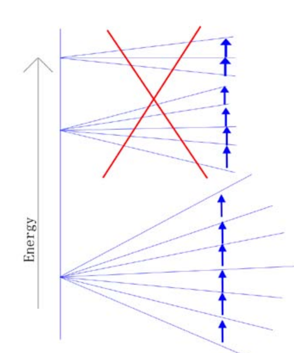
Introduction

Single molecule magnets (SMM) have potential applications in quantum computing and data storage. Recently fabricated 4f-3d compounds have been demonstrated to show SMM behavior[1] but the mechanism for this has yet to be understood.



- Determine magnetic properties of several rare earth based molecular magnets of 4f-3d structure
- Test newly formulated Ising-model spin Hamiltonian
- Analyze exchange coupling between 3d and rare earth (4f) ions

$$\hat{\mathcal{H}} = -J\sum_{i=1}^{n}\hat{J}_i^z \cdot \hat{S}^z + \mu_B H^z (g_{Dy}\sum_{i=1}^{n} J_i^z + g_{Cu}S^z) + \mathcal{H}',$$



Recently developed Ising-model spin Hamiltonian for determining energy of 4f-3d systems at low temperatures[1]

1. Hiroyuki Nojiri et al., J. AM. CHEM. SOC. **2006** *128* (5), 1440-1441

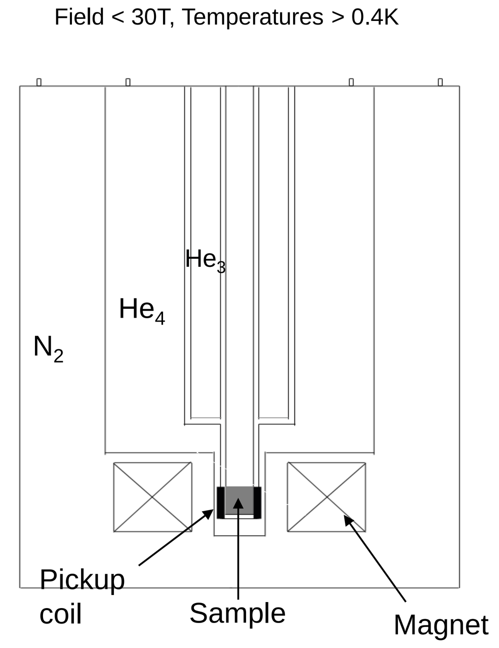
Single molecule magnet (SMM)- molecule that behaves as an independent tiny magnet

Application and removal of magnetic field

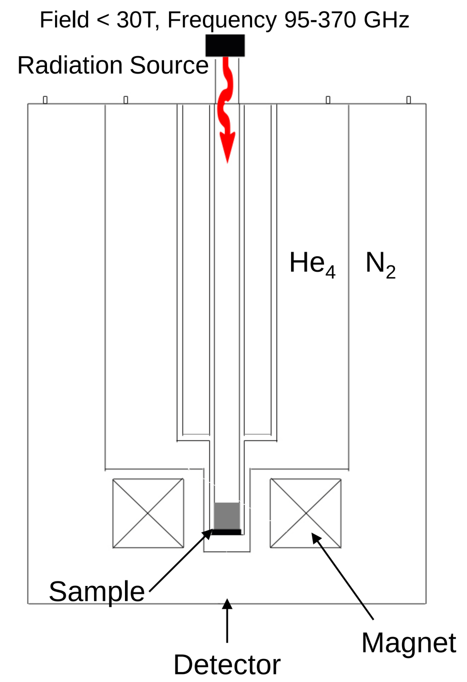
Method

- EPR and Magnetization of four novel 4f-3d samples
- Determine state/ exchange coupling
- Compare with other 4f-3d structures

Magnetization
Field < 30T, Temperatures > 0.4K

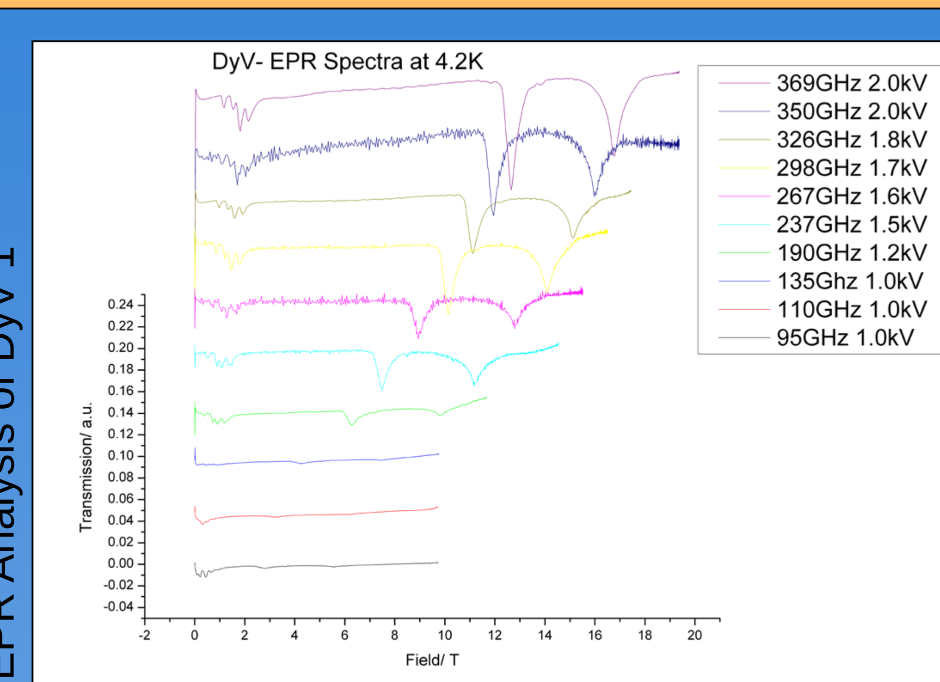


ESR
Field < 30T, Frequency 95-370 GHz

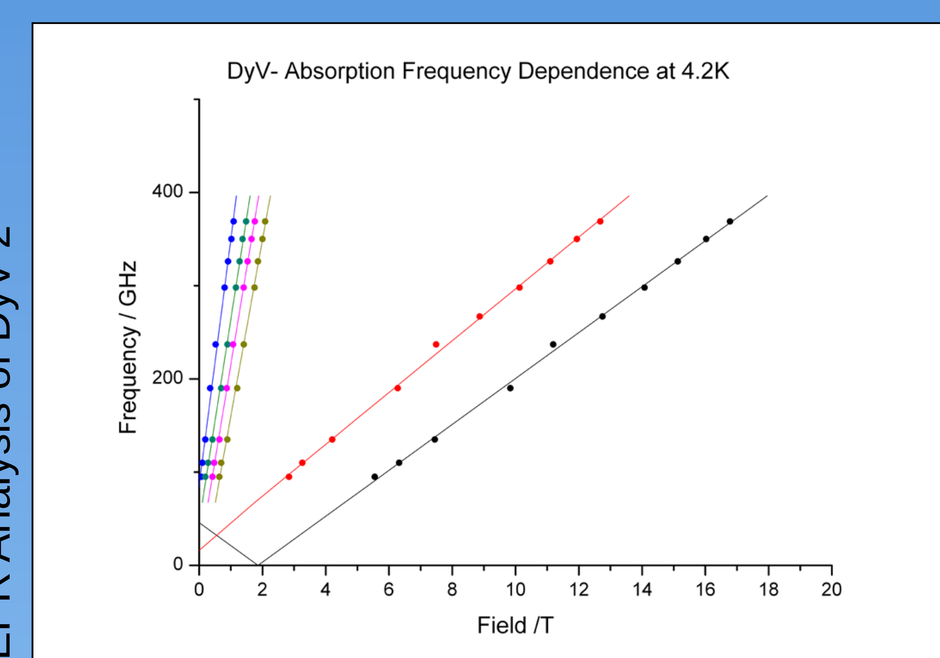


Results

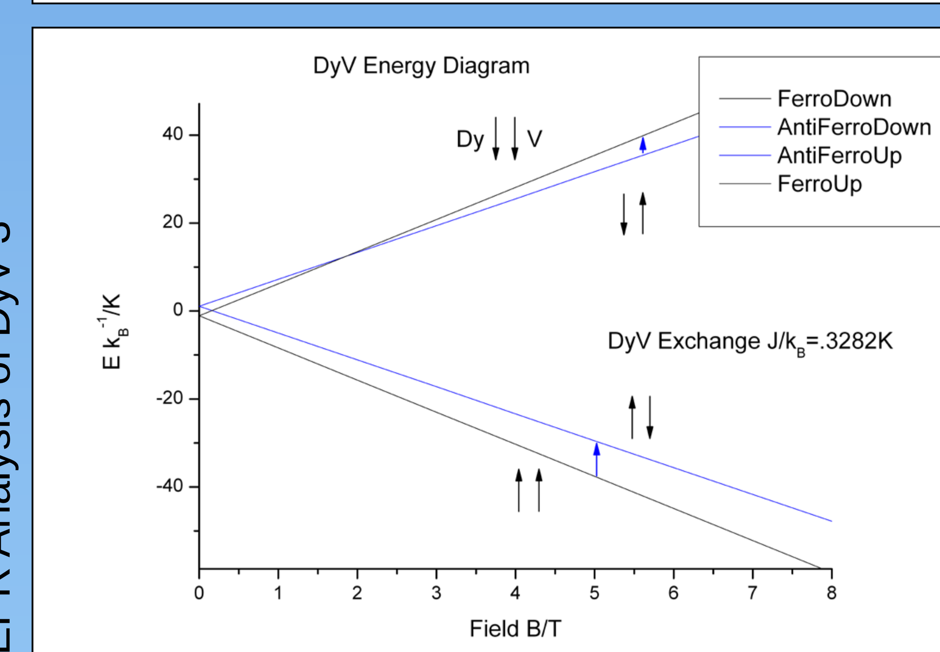
EPR Analysis of DyV 1



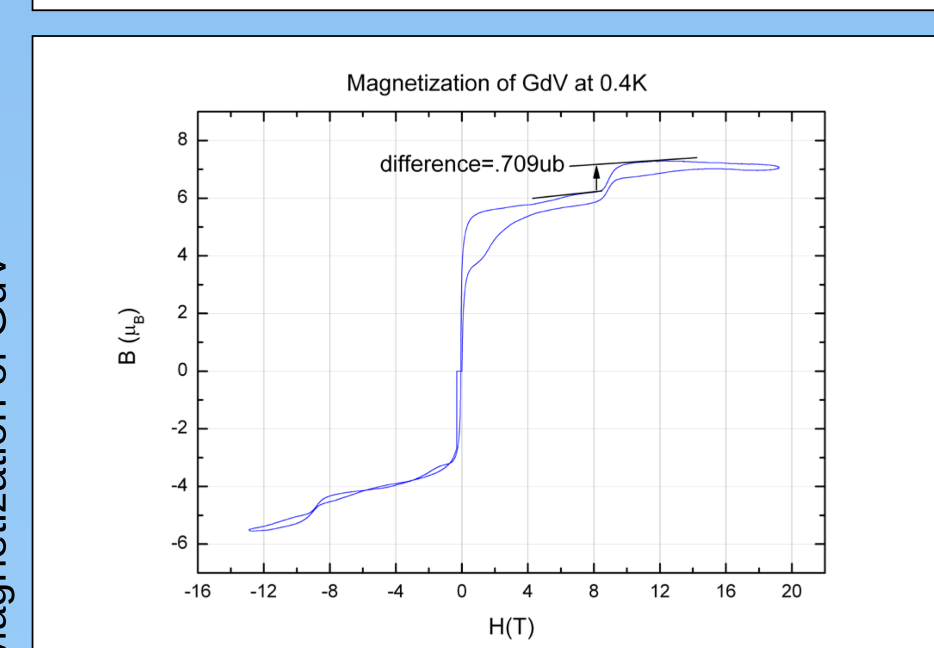
EPR Analysis of DyV 2



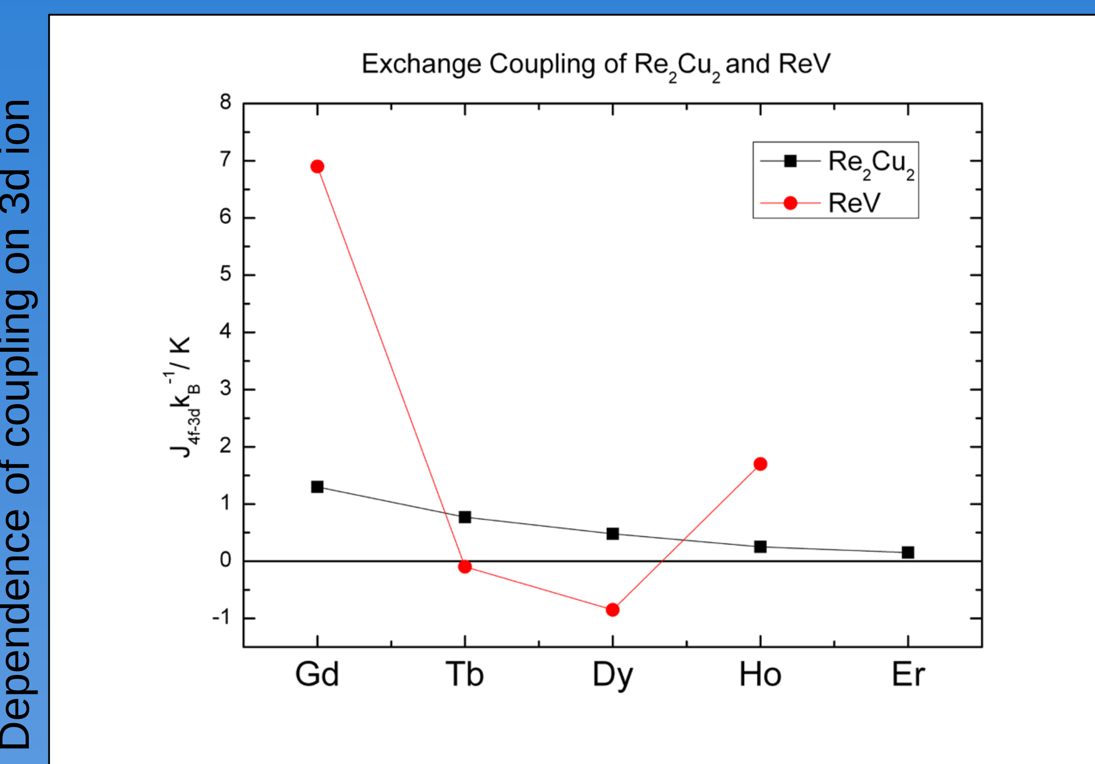
EPR Analysis of DyV 3



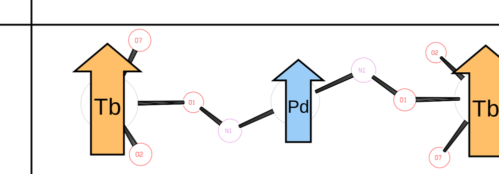
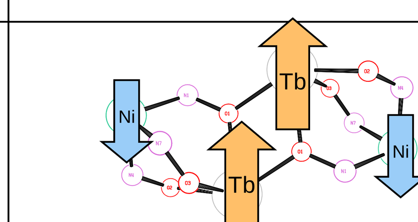
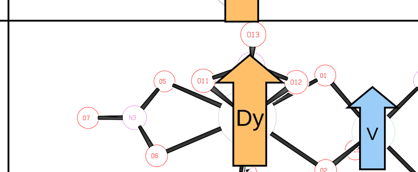
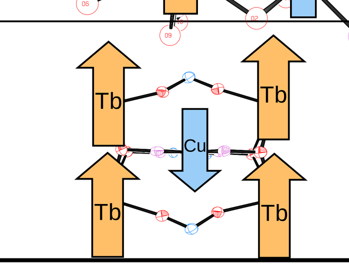
Magnetization of GdV



Dependence of coupling on 3d ion



Characterization

Sample	State*	Exchange (K)*	Bond Length(Å)	J Moment	Crystal Structure (4f-3d atoms and ligands only)
TbPdTb	Ferro	-0.442	4.79	5	
Tb_2Ni_2	Ferri	-0.077	3.95	5	
DyV	Ferro	0.328	3.49	15/2	
Tb_4Cu	Ferri	0.92	3.76	5	

*Determined by our experiment

Conclusions

- Ground state and coupling constant between the 4f-3d ions determined.
- The spin Hamiltonian successfully modeled the energy levels of the samples.
- The exchange constants were compared with previous samples, showing the dependency of coupling on the valence shell of the 3d ion in 4f-3d samples.
- GdV was determined to have the largest exchange coupling constant of any SMM to date. This has the potential for fabrication of an ultra-high spin single molecule magnet.

In the future, more isomorphic 4f-3d samples can be tested to further validate the spin Hamiltonian and to further analyze coupling in such compounds.

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http://nanojapan.rice.edu

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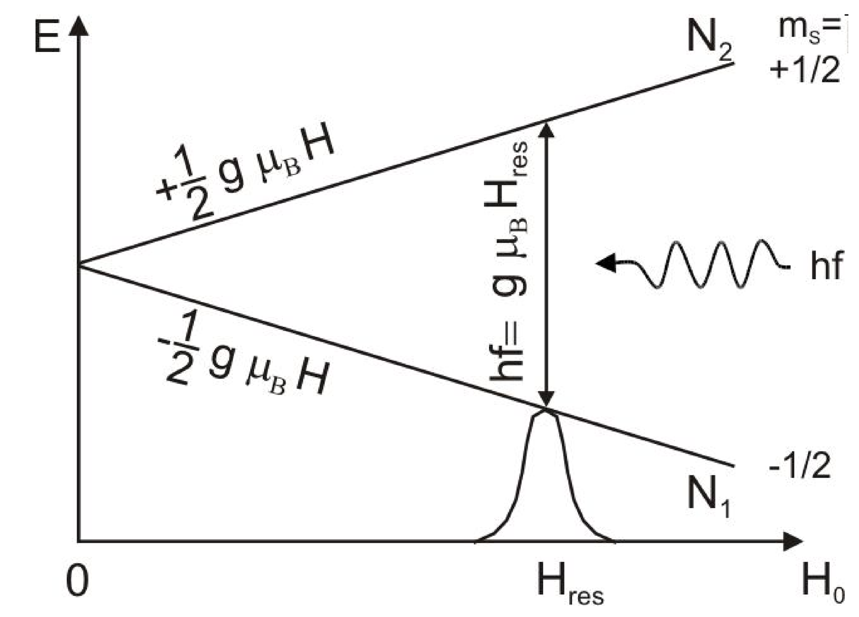
$$B_J(x) = \frac{2J+1}{2J}\coth\left(\frac{2J+1}{2J}x\right) - \frac{1}{2J}\coth\left(\frac{1}{2J}x\right)$$

$$M = Ng\mu_B J \cdot B_J(x)$$



$$\vec{\mu} = -\mu_B g \vec{J}/\hbar,$$