

Magnetic properties of Erbium metal coordination complexes

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ABSTRACT: Certain lanthanide containing coordination complexes give rise to magnetic properties that may make them useful as storage devices. This study focuses on the synthesis of single ion magnets (SIMs) that are specifically coordination complex molecules that contain central Erbium lanthanide metals. The ligand that we used in this study is H_2ovph . In order to form this molecule we combined Erbium metal with the ligand in their respective solvents for coordination complex formation. In order to achieve the desired SIM, we controlled certain factors of the reaction (such as the solvents being used) in order to ultimately produce perfect conditions for the coordination complex to form. Upon attaining the desirable molecule, we tested its magnetic properties. Our final results did not confirm SIM properties for the molecule.



ErCl₃

Procedure:

Much of this investigation comprised of idealizing the environment of the reaction of our ligand, H_2ovph , with $ErCl_3$ (Erbium chloride). Two equivalents of the base $NaHCO_3$ was used to neutralize the ligand. In order to idealize the conditions, different types of solvents were used until favourable solvents were found. Methyl Cyanide was consistently used for the organic ligand and the base, due to its ideal properties in the formation of coordination complexes. 5mL of isopropyl alcohol and 2mL of 2,5-dimethylformamide (DMF) was used for the Erbium metal for the formation of the complex.

It was vital to add DMF to isopropanol for the metal to fully dissolve. This was done to ensure sufficient reaction of the metal with the ligand. After complete dissolving of the metal in the solvent, we added the dissolved metal to the ligand solution. A magnetic stirrer was used to effectively dissolve the reactants, particularly the metal in its solvent. Stirring was continued for forty minutes.

After 40 minutes, the solution was filtered and left to crystallize. The crystals appeared like thin needles that were uniformly suspended in the solution. The crystal was then analyzed by means of single X-ray crystallography and IR (Infra-Red) to understand its structure. Finally to determine the magnetic properties of the coordination complex, SQUID was used. SQUID is a superconducting quantum interference device.

References and Acknowledgements:

Guo, Yun-Nan, Xu, Gong-Feng, et al. "Strong Axiality and Ising Exchange Interaction Suppress Zero-Field Tunneling of Magnetization of an Asymmetric Dy₂ Single-Molecule Magnet." *Journal Of The American Chemical Society*. 133.31 (2011): 11948–11951. Print.

Walkerma, . *Erbium(III)chloride_sunlight.jpg*. N.d. Photograph. WikipediaWeb. 21 Mar 2014. <[http://en.wikipedia.org/wiki/File:Erbium\(III\)chloride_sunlight.jpg](http://en.wikipedia.org/wiki/File:Erbium(III)chloride_sunlight.jpg)>.

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Introduction:

Magnetic storage involves medium that have magnetic properties that give rise to their ability to store non-volatile data. Some examples of this means of data storage are hard disks, floppy disks, and the magnetic stripe of a credit card. Specifically, single-ion magnets (SIMs) can be produced to perform this function. This is attempted to be produced in the experiment.

In this project, we aimed to develop a single-ion magnet involving a coordination complex which is made up of a ligand and central lanthanide metals. A coordination complex is a molecule containing central metal atoms with a surrounding organic ligand whose electrons interact with the central metal. The lanthanide metals make up a row of elements in the periodic table and are distinguished by common characteristics that include high reactivity, binding with water, strongly reducing nature and high melting and boiling points. More importantly, lanthanide single-magnet ions have slow magnetization relaxation. This is a vital characteristic that is required for a reliable memory storage device.

A previous investigation with regards to lanthanide coordination complexes has been successful in determining its slow magnetic relaxation behaviour (Guo, Xu, et al., 11948-11951). This was done with Dysprosium as the central lanthanide metals. Therefore we are optimistic that other lanthanides can also exhibit this behaviour. Specifically, this investigation is based on determining the magnetic properties of a coordination complex that is made up of the ligand H_2ovph and the Erbium lanthanide metal. Erbium has similar properties to Dysprosium, with a similar electron configuration. It usually occurs in ionic compounds such as in $ErCl_3$ which is what was used in this study.

Results:

Information on the coordination complex including its structure and magnetic properties were obtained with IR, single X-ray crystallography and SQUID. The following Infra Red spectrum was taken of the Erbium coordination complex formed from this experiment.

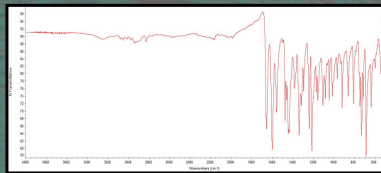


Figure 1. IR spectrum for erbium coordination complex with H_2ovph .

Single X-ray crystallography was used to determine the exact structure of the coordination complex and also other qualities of the molecule that are summarized in the table below.

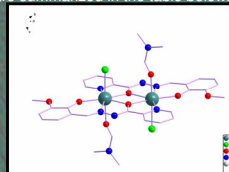


Figure 2. Structure of the erbium coordination complex through visualization with single X-ray crystallography.

Identification code	Empirical formula	Formula weight	Temperature	Wavelength	Crystal system	Space group	Unit cell dimensions	Volume	Z
Mm331	C34 H38 Cl2 Er2 N8 O8	1092.14	200(2) K	0.71073 Å	Monoclinic	P 21h	a = 9.22190(10) Å b = 11.9769(2) Å c = 97.7980(8)° β = 17.4808(3)° α, γ = 90°	1912.90(5) Å ³	2

Figure 3. Information on complex that was retrieved from X-ray crystallography.

SQUID was used to analyze the magnetic properties of the sample. The following graphs illustrate magnetic properties of the Erbium coordination complex.

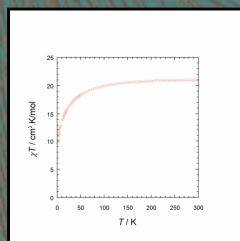


Figure 4. Temperature dependence of the χMT products at 1000 Oe for $Er(III)$ complex. The antiferromagnetic interaction has been shown. At 300 K, the χMT value is 20.9662 $cm^3 K mol^{-1}$, which is lower than the theoretical value of 22.95 $cm^3 K mol^{-1}$ for two noninteracting $Er(III)$ ions ($4f^{15/2}$, $s=5/2$, $\chi_T = 11.48 cm^3 K mol^{-1}$).

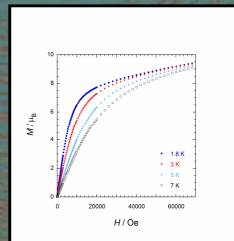


Figure 5. Field dependence of the magnetisation for $Er(III)$ complex at indicated temperatures. Figure 1.

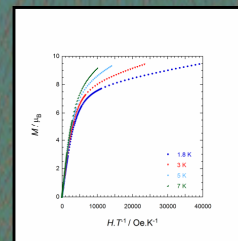


Figure 6. M vs. HT^{-1} plot for $Er(III)$ complex at indicated temperatures. The high-field variation and lack of a clear saturation of the M vs HT^{-1} data suggest the presence of a significant magnetanisotropy and/or low-lying excitation states present in the molecule.

Conclusion:

According to the Infra Red Spectrum, the stretch that occurs at around $1660cm^{-1}$ represents the double bond of a carbonyl in the amide group of DMF. Also, the peaks that occur from $1550-1600cm^{-1}$ represent C=C bonds in aromatic rings that occur in the structure of the ligand H_2ovph . The IR of this molecule shows that some DMF has bonded to the coordination. It clearly indicates the presence of the ligand in the molecule. Although the IR does express some indication of a coordination complex formation, it does not confirm that the molecule is the desirable complex and an X-ray is vital to confirm this.

The X-ray shows that the chemical formula of the molecule includes both the atoms of the ligand and two erbium atoms. The image of the X-ray shows that the molecule is the desired structure that includes two central lanthanide atoms being surrounded by the ligand. This molecule resembles the Dysprosium containing coordination complex that has been proven to express slow magnetization relaxation (Guo, Xu, et al., 11949).

Finally the graphs that demonstrate the results from the SQUID device reveal that the coordination complex does have some magnetic properties. For instance, the coordination complex has some magnetic properties according to Figure 5 which illustrates its increasing dependence on a magnetic field to retain its magnetization with the increase of temperature. However, the molecule can not be classified as a Single Ion Magnet for factors such as the value of χ^{MT} at 300K which is not the literature value for at that temperature for two interacting Erbium atoms (Figure 4). The reaction should be repeated and potentially be tested with another solvent in the future.