Introduction:
Clusters of transition metals have attracted much interest from the chemical society and other interdisciplinary research fields. Polynuclear complexes of Fe and Mn have proven interesting due to their magnetic properties. Usually, such clusters exhibit large ground-state magnetic moments and can function as single-molecule magnets due to a high energy barrier to magnetization relaxation. Thus, such molecules can retain magnetic orientation for prolonged periods of time without further addition of energy. These molecular systems have potential application to molecular data storage devices.

To further increase the functionality of such compounds, redox-active ligands have been introduced to the cluster core. For the scope of this research, ferrocene-1,1’-dicarboxylic acid (FdcH₂, Figure 1) was used as a base for carboxylate ligation within the cluster. The premise of my work was based on previous publication describing Mn and Fe clusters, more specifically an ionic Fe₇Cl₂ cluster, which also utilized FdcH₂ as a redox-active ligand. Redox-active ligation with FdcH₂ is important for data storage devices since the dicarboxylate anion can undergo reversible one-electron reduction/oxidation chemistry. It can also act as a restrictive bridging ligand or chelate with regard to molecular flexibility, however, it can retain rotational properties of its cyclopentadienyl rings to further bridge other units leading to polymers.

Figure 1: Molecular structure of ferrocene-1,1’-dicarboxylic acid (FdcH₂).
The purpose of this research was to find and optimize synthetic conditions for a neutral mixed-valent state cluster via dicarboxylate ligation.

Materials and Methods:
Synthesis: Several experimental conditions were explored:

- Visible Polymers (Brown)
- Invisible Polymers (Brown)

X-ray Crystallography: X-ray diffraction data were collected on a Rigaku RAPID II diffractometer with a curved detector using graphite monochromated Mo-Kα (λ = 0.71073 Å) at 123 K. Multi-scan absorption corrections were applied to the data using the Crystal Clear program. The structures were solved by direct method implemented in SHELXS-97 and refined by full-matrix least squares method based on F2 using SHELXL-97 software. PLATON software was used for visualization of the results.

Elemental Analysis: Analysis performed by Atlantic Microlab, INC. Analyzed for C, H, and N.

Discussion:
The purpose of this experiment was to optimize-synthetic condition of a neutral Fe₇O₇ cluster based on previous reported results. Crystallographic analysis supported the presence of an Fe₇O₇ cluster, revealed Fe(II) and Fe(III) atoms within the cluster. Furthermore, it was deduced that the presence of Fe(II) and Fe(III) in the cluster is attributed only to a decomposition, via solvolysis, of FdcH₂. The color change from orange (initial solution of FdcH₂ in MeOH) to dark-blue (final product) can be attributed to the one electron oxidation of Fe(III) to Fe(II).

The crystal structure of the Fe₇O₇ cluster is better described as a combination of the inorganic and organic moieties. Thus, the inorganic core consists of cubane Fe₅O₆, formed from four hexacoordinated Fe(III) ionic nature, more specifically, when analyzing magnetic properties of their compound, the paramagnetic effects of the cluster. Fe(II), Fe(III), and the cluster became evident. However, one similarity between our work and Masello et al. on their synthesis of a cationic species expressed problems regarding the characterization of the compound due to its composition. ic properties of its coordination: neutral cluster (FeCl₃) is formed from four Fe(III) ions, which can be separately oxidized with regard to the driving force of this reaction. The relevance of such compound to data storage lies within its ferrocene substituents which can be separately oxidized in six different oxidation potentials.

In the future, I hope to perform Powder diffraction, Mössbauer Spectroscopy, and Electron Paramagnetic Resonance (EPR) to further characterize the compound. Further research could also include experimentation with other alcohols.

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