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# Increased Order in Single Molecule Magnets

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#### Abstract

Single Molecule Magnets (SMMs) show promise in advancing computer technology and our understanding of quantum behaviours, however we first have to understand how to successfully synthesize ligand systems that allow them to perform at viable temperatures. As such, my project explored the synthesis of new ligand systems for potential SMMs based on [2.2]paracyclophane and pyrazine. These structures were chosen to be a synthetic backbone for the synthesis of new ligands for potential SMMs formation due to their structural and electronic properties. Attempts were undertaken to form complexes with these ligands and grow crystals suitable for X-ray crystallography.

In this project three new ligand systems were synthesized and characterized, one with a [2.2]paracyclophane backbone ( $\mathbf{L}_1$ ) and two containing a pyrazine bridging group ( $\mathbf{L}_2$  and  $\mathbf{L}_3$ ). Complexations with a variety of metals were undertaken with all three ligands, unfortunately crystals of sufficient quality for single crystal X-ray diffraction experiments were not obtained. In total 8 new compounds were synthesized and a novel route for the synthesis of 4-(benzylamino)[2.2]PC was developed during this project.

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#### **Abbreviations**

[2.2]PC [2.2]Paracyclophane

AC Alternating Current

Ac Acetyl

BINAP 2,2'-Bis(diphenylphosphino)-1,1'-binapthyl

Bn Benzyl

dba Dibenzylideneacetone

DC Direct Current

DCM Dichloromethane

DMF Dimethylformamide

DMSO Dimethyl sulfoxide

EDTA Ethylenediaminetetraacetic acid

Et Ethyl

H External magnetic field

K Kelvin

m-CPBA meta-Chloroperoxybenzoic acid

Me Methyl

NBS *N*-Bromosuccinimide

NMR Nuclear Magnetic Resonance

Ph Phenyl

QTM Quantum Tunnelling of Magnetism

RT Room Temperature

S Spin state

sao Salicylaldoxime

SMM Single Molecule Magnets

T Tesla

T<sub>B</sub> Blocking temperature

THF Tetrahydrofuran

TLC Thin Layer Chromatography

Ts 4-toluenesulfonyl

 $U_{
m eff}$  Thermal barrier

 $X_m$ " Out-of-phase component