Synthesis of a Mechanically Active Gadolinium Chelate

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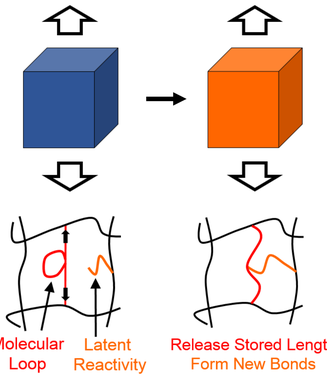
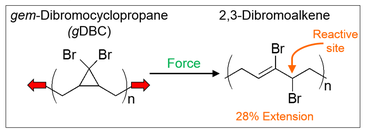
Introduction

A mechanophore is a chemical functional group that is activated by mechanical force.[1]

- Produces color change, fluorescence, small molecule release
- Applications in sensors, data displays, self-strengthening materials

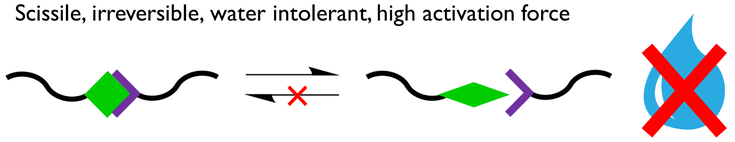


Example:



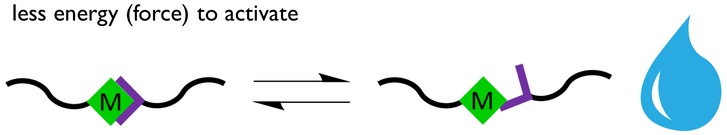
Project Design

Problems with most current systems:
Scissile, irreversible, water intolerant, high activation force



Organometallic complexes could solve these problems:

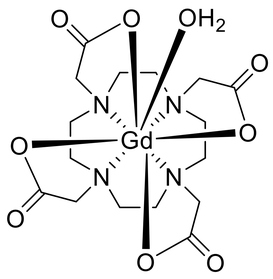
Metal-ligand bonds are weaker than organic covalent bonds, requiring less energy (force) to activate



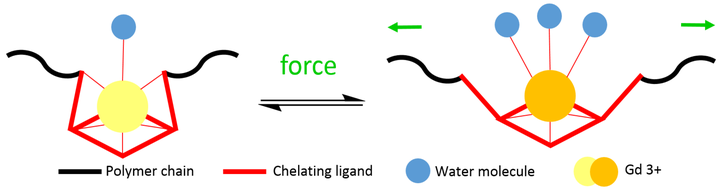
Magnetic Resonance Imaging (MRI) contrast agents provide an excellent chelate design[3] which can be modified to act as a mechanophore.

Strategy:

1. Complex incorporated into polymer backbone
2. Force applied to bulk polymer
3. Force transferred from polymer to complex
4. Parts of ligand dissociate
5. Solvent (water) coordinates in their place
6. Change in coordination sphere = change in color



Gadoteric acid[3]
Commercial MRI Contrast Agent



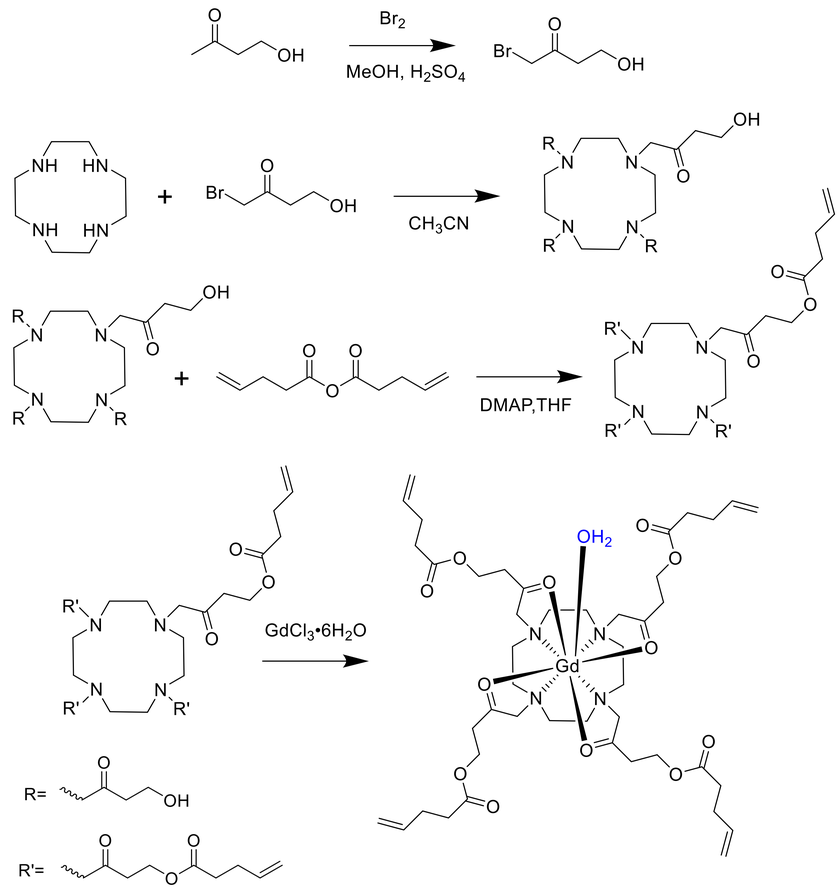
Goals

A) Design a metal complex as an effective mechanophore that changes color under applied force as a colorimetric tension sensing system.

B) Synthesize the target mechanophore and perform mechanical testing.

A successful project would provide proof of concept for a totally new class of mechanophore.

Synthesis



Reaction conditions optimized and monitored by ^{1}H NMR. Absorbance, excitation and emission data will be collected on the final complex by UV-Vis spectroscopy. Synthesis based off sources 5,6.

References

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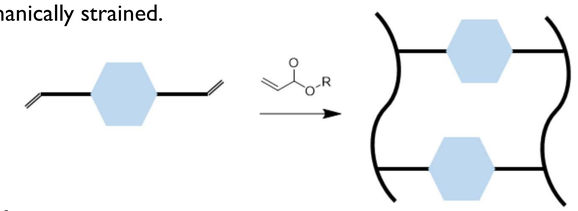
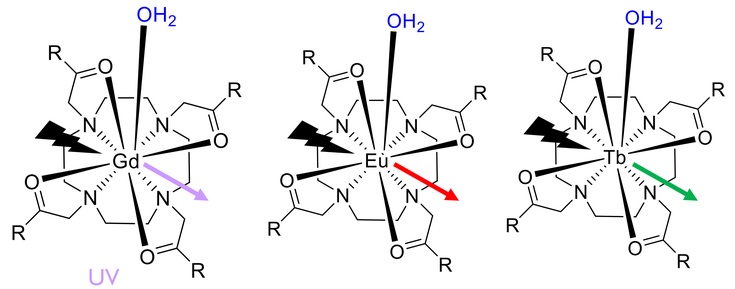
Future Work

Upon successful synthesis of the target compound, it will be incorporated into a hydrogel as a load-bearing cross-linker which will then be mechanically strained.

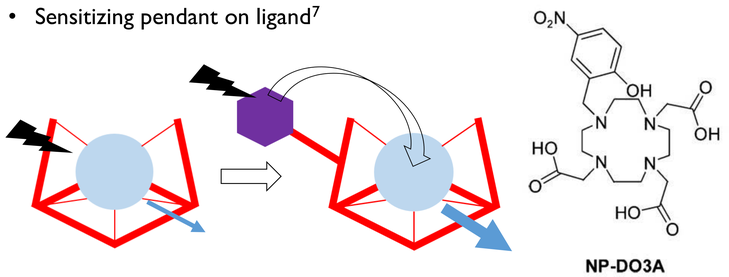


Modifications:

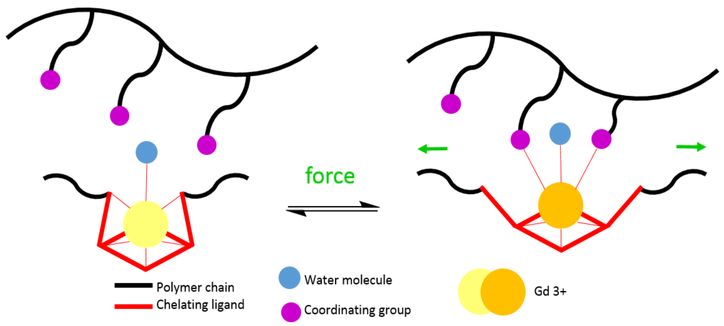
- Different metal[5]; Europium (Eu), Terbium (Tb)



- Sensitizing pendant on ligand[7]



Incorporation of this complex into a different polymer, for example one that had dangling amine groups, could facilitate cross-bridging upon the application of force. The goal of this would be to create a self-strengthening material.



Acknowledgements

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