



#### Introduction

Silatranes are well-known compounds containing a transannulardative bond between a nitrogen and silicon atom in a tricyclic compound. Using an easily interchangeable functional group on the silicon atom, they have been used in a wide amount of fields from medicines to industrial adhesives.<sup>1</sup> However, while substituent groups attached to the silicon atom have been the focus of much research with regard to its affect on the dative bond in the molecule, little research has been done at the opposing end, using the nitrogen to influence the bond.<sup>2</sup>

Ongoing research is currently being done in pursuing the synthesis of 1-methyl-4silatranone to see the effects of adding a carbonyl to the carbon alpha to the nitrogen atom. Theoretical calculations lead to the notion that an anti-Bredt conformation is obtained where there is a double bond at a bridgehead due to the molecule being a hyperstable lactam.<sup>3</sup> Multiple pathways have been investigated to find the proper conditions for synthesizing 1-methyl-4-silatranone. Multiple pathways include coupling reactions, acetonide precursors, and most recently a pseudosilatrane route in which the closing and creation of an amide is the final step in closing the tricyclic silatranone.



Scheme 1. Both Trial Pathways

#### **Synthesis of N-glycolyl-diethanolamine**

The following reactions describe the synthesis of N-glycolyl-diethanolamine which is a precursor for the synthesis of 1-methyl-4-silatranone via path A.



# The Investigation of the Synthesis of 1-Methyl-4-Silatranone

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Figure 1. Standard Silatrane

# **Synthesis of Pseudosilatrane**

The following reactions describe a synthesis of pseudosilatrane which is a precursor for the synthesis of 1-methyl-4-silatranone via path B. The pseudosilatrane route involves first making the bicyclic pseudosilatrane using diethanolamine and triethoxymethyl silane while vacuum distilling ethanol to force the generation of product. The second step requires adding ethylene glycol under similar conditions to attach the final substituent.<sup>4</sup>



Pseudosilatrane precursor

## Discussion

After multiple trials using *N-glycolyl-diethanolamine* to try and synthesize the silatranone, it was thought the dative bond in a silatrane is one of the main driving forces that allows the reaction to occur.<sup>5</sup> Due to the hypothesized structure of the silatranone, it lacks the dative bond between the nitrogen and the silicon atom, thus, forming a silatranone via silatrane mechanisms may not be feasible. Thus, it was thought that making the bicyclic pseudosilatrane first, and closing the silatranone using an oxidation reaction and coupling reaction, would be much more energetically favorable.

## **Future Work**

Due to the recent considerations of the energies of the mechanism, not a large amount of work has been put into trial in the synthesis of a silatranone via pseudosilatanes. Future work includes researching more on the, already known, pseudosilatranes, as well as making attempts at the synthesis and analysis of 1-methyl-4-silatranone or it's many derivatives.

## Conclusions

Overall, good progress has been made in forming precursors to 1-methyl-4silatranone. In addition, many trials, and understanding of pathways also have helped in understanding the nature of both silatranes and silatranones.

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