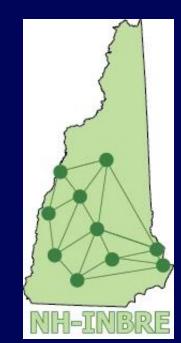


Synthesis of 1,3,5,7-tetraethynyladamantane

Timothy J. Cooke, Dr. Carolyn Weinreb Department of Chemistry, Saint Anselm College 100 Saint Anselm Drive, Manchester, NH 03102





Abstract

Four of the first five steps of the synthesis of 1,3,5,7-tetraethynyladamantane were completed and confirmed by IR or NMR with a yield of 21%. As a model system, 1-ethynyladamantane was used for the synthesis of 1,3,5,7-tetraethynyladamantane. Adamantanealdehyde (4) was prepared with a 47% yield.

Introduction

- The overall goal of the project is a more efficient synthesis of 1,3,5,7-tetraethynyladamantane.
- The current published synthesis of this product is 9 steps with an overall yield of 11%.¹
- Terminal alkynes are useful in organic synthesis because they can undergo a large number of reactions, such as nucleophilic or electrophilic addition, hydroboration-oxidation, hydration, reduction, or organometallic coupling reactions.²
- This versatility would allow the molecule to be functionalized in a large number of ways.
- The structure of 1,3,5,7-tetraethynyladamantane potentially has interesting characteristics, such as being able to form 3D polymers and its potential to conduct electricity.
- As a model for the tetra-substituted product, the synthesis of 1-ethynyladamantane was chosen.

2. Loudon, M., Organic Chemistry. 5th ed.; Roberts and Co.: Greenwood Village, CO, 2009. 644-675

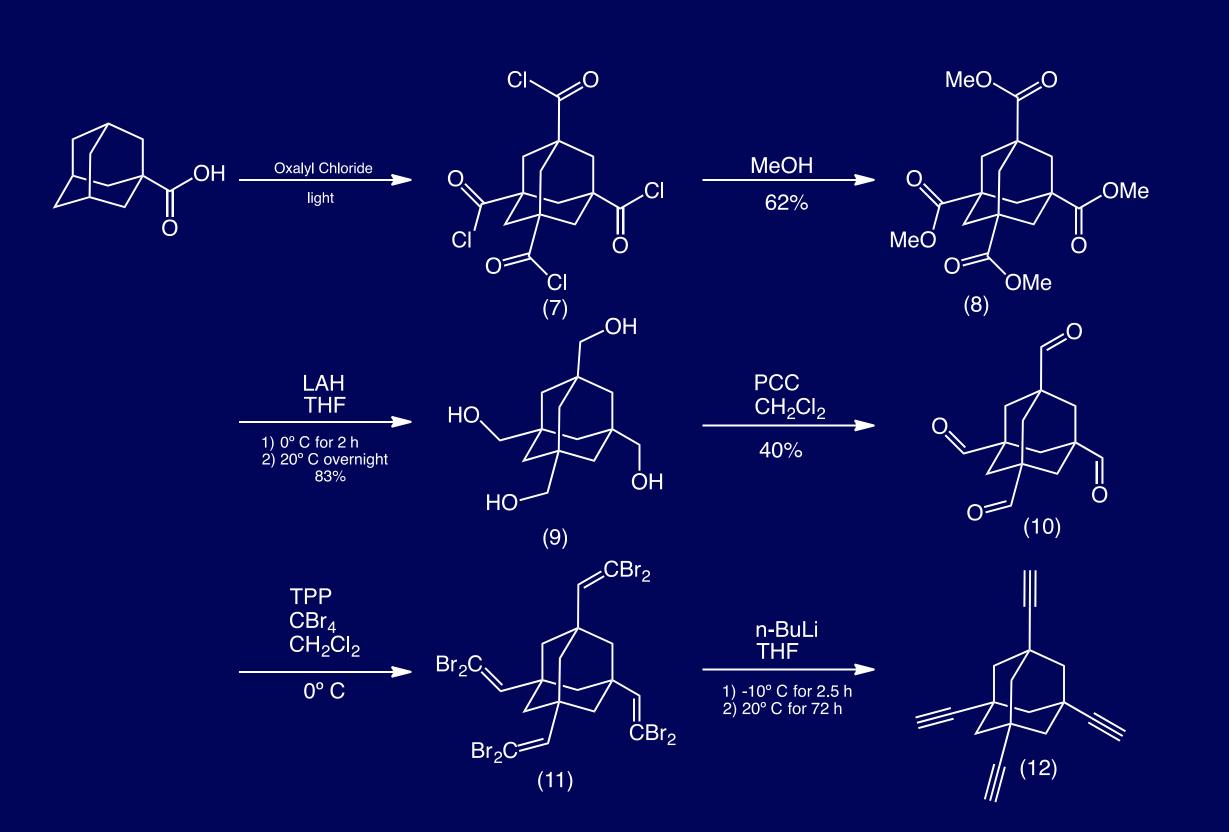
References

1. Naemura, K.; Hokura, Y.; Nakazaki, M., Synthesis of (+)-1,3,5,7-tetrakis[2-(1S,3S,5R,6S,8R,10R)-D3-trishomocubanylbuta-1,3-diynyl]adamantane. *Tetrahedron* **1985**, (42), 1763-1768.

Methods

Synthetic Pathway for 1-ethynyladamantane

Synthetic Pathway for 1,3,5,7-tetraethynyladamantane



Results/Discussion

- 1-ethynyladamantane was synthesized and characterized through the first four steps of the reaction and it was determined that the yield to that point was 47%
- 1,3,5,7-tetraethynyladamantane was synthesized and characterized through the first four steps as well, and it was determined that the yield to this point was 21%.

Conclusions

- While neither product was fully synthesized, four of the five steps in the proposed reactions were completed and characterized by either NMR or IR spectroscopy.
- The proposed synthetic pathway is viable as a more efficient synthesis of these compounds.

Acknowledgements

• I would like to thank Mark St. Peter and Sarah Wojtas for their previous work on this project and I would like to thank Dr. Weinreb for her guidance and patience.

Funding

This project was funded by NH-INBRE