Synthesis of Substituted Pyrazoles and Imidazolium Salts

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Introduction

- Pyrazoles and imidazolium salts are heterocycles that contain nitrogen atoms.
- This research project concentrates on synthesizing substituted pyrazoles and imidazolium salts as precursors to desired ligands.
- The ligands can then be used in lactide polymerization to create poly-lactic acid, a biodegradable alternative to polyethylene.

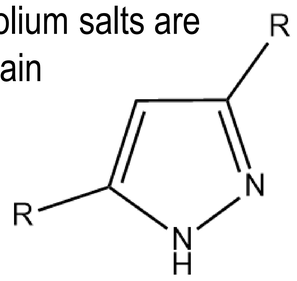


Figure 1: *Structure of a disubstituted pyrazole*

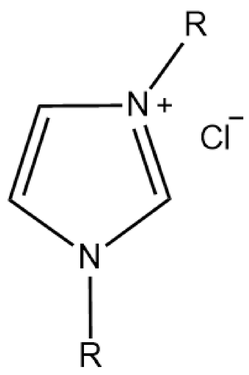
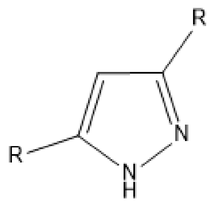


Figure 2: *Structure of a disubstituted imidazolium chloride salt*

Results and Analysis



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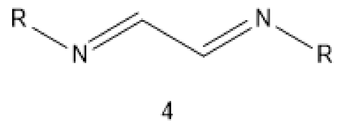

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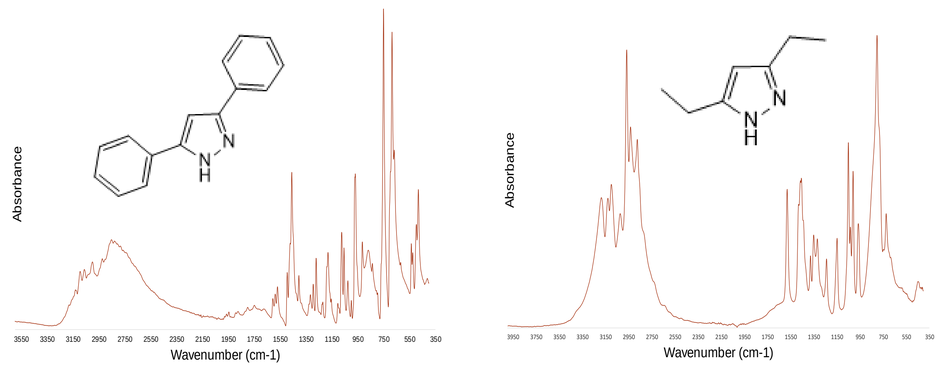
Target Molecule	R-group	Percent Yield
2A	Ethyl (CH_2CH_3)	72%
2B	Phenyl (C_6H_5)	58%
4A	Tert-butyl ($C(CH_3)_3$)	8%
4B	Phenyl (C_6H_5)	91%
4C	Adamantyl ($C_{10}H_{15}$)	39%

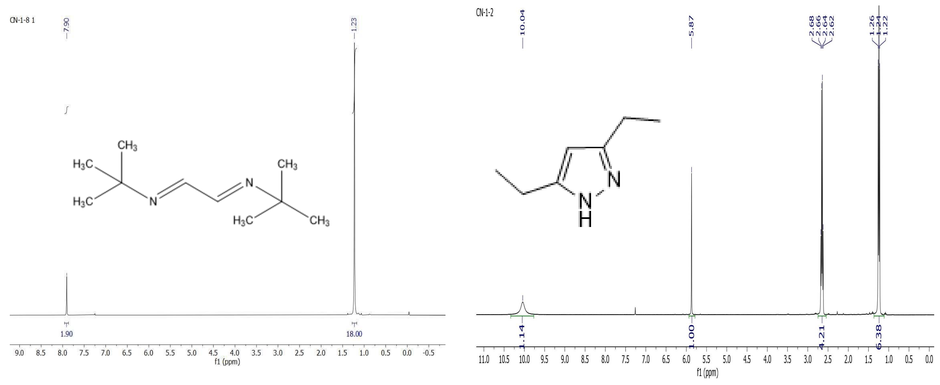
Table 1: *Percent Yields of Disubstituted Pyrazoles and Diimines*

- Infrared (IR) and nuclear magnetic resonance (NMR) spectroscopy were used to analyze and confirm the synthesis of the target molecules.

IR Spectroscopy

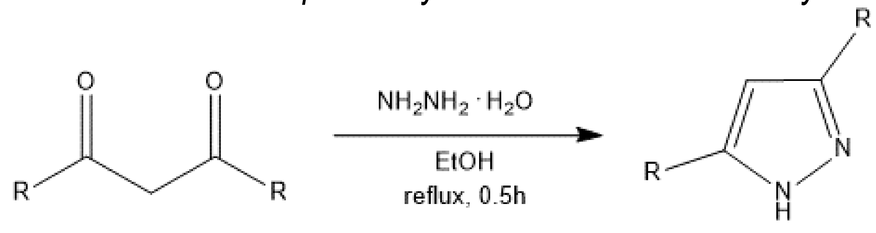


NMR Spectroscopy



Synthetic Routes

Reaction Scheme 1: *Proposed Synthesis of Disubstituted Pyrazoles*



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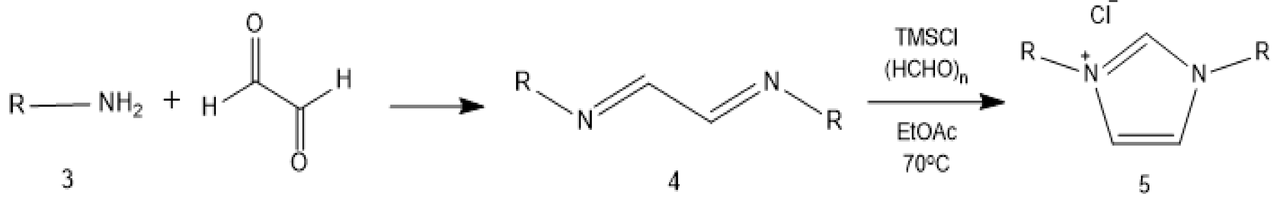
A: R=ethyl (CH_2CH_3)
B: R=phenyl (C_6H_5)

Reaction Scheme 2: *Proposed Synthesis of Disubstituted Imidazolium Chloride Salts*



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A: R=tert-butyl ($C(CH_3)_3$)
B: R=phenyl (C_6H_5)
C: R=adamantyl ($C_{10}H_{15}$)

Next Steps

- Synthesis of other substituted pyrazoles and diimines
- Improvement of the imidazolium salt reactions to obtain better yields and/or purer product

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