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Senior Project Title: Accessing diynes containing thiocyanate end-groups en route towards polydiacetylenes

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Major: Chemistry

### Abstract

The synthesis of diynes with sulfur-containing end groups was explored en route towards accessing novel polydiacetylenes (PDAs), a class of conjugated polymers with conductive properties. Diynes containing thiophene and thiocyanate end-groups have been targeted, with the latter being the focus of this project. Thiocyanate (SCN) end-groups are expected to impact the electronic properties of the polymerized system because of the resonance-stabilization and electronic effects of these groups. Efforts to synthesize 1,4-dithiocyanatobuta-1,3-diyne have yielded promising results, with  $^{13}\text{C}$  NMR data containing peaks that correspond well with predicted spectra. Additional characterization is needed to confirm isolation of this novel diyne before polymerization can be fully explored. Computational simulation of chemical shifts was explored to complement the experimental and predicted NMR spectra. Removal of trace solvents such as triethylamine has proven troublesome, thus complicating initial polymerization efforts. However, recent spectroscopic data indicates successful isolation of the diyne that would facilitate future polymerization attempts.

