

## ABSTRACT

## Exploring New Techniques For Precision Deuteration of Alkenes and Alkynes

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Deuterium labeled compounds are often utilized in chemical research as internal standards in mass spectrometry, to study reaction mechanisms and in the pharmaceutical industry to slow the rate of metabolism. With the increase interest for deuterium labeled molecules, there is a renewed interest in selective methods for the installation of deuterium atoms into small organic molecules. However, current methods to incorporate deuterium atoms into organic molecules can lead to isotopic mixtures such as isotopologues and isotopomers. These isotopic species are indistinguishable due to their similar physical properties, leading to inseparable products by common purification techniques. Furthermore, common spectroscopic techniques to specifically characterize and measure the precise location of the deuterium atom and sample composition of isotopic species are deficient.

Catalytic transfer hydrodeuteration and deuteration reactions are emerging powerful techniques for site-selective and chemo-selective reactions to install deuterium atoms into small molecules. This method offers advantageous opportunities to improve selectivity and access precisely deuterated molecules as it offers tunable reaction conditions and tolerates a broad substrate scope. Additionally, this method uses inexpensive, readily available, easy to handle deuterium donors precluding the need of highly flammable deuterium gas. Herein, methods to precisely install deuterium atom(s) in a single step across alkene and alkyne functionalities under copper-catalyzed transfer deuteration and hydrodeuteration conditions are described. In this dissertation, reactivity, regioselectivity, and enantioselectivity is investigated.

Molecular rotational resonance (MRR) spectroscopy is also employed for characterization of possible isotopic species present in the reaction mixture from Cu-catalyzed transfer hydrodeuteration reactions. Through MRR spectroscopy, confirmation of regioselectivity was acquired and any possible isotopologues and isotopomers were quantified. Lastly, by using chiral tagging in MRR spectroscopy, we report the first general spectroscopic technique for enantiomeric excess and absolute configuration determination of chiral by virtue of deuterium substitution compounds synthesized by a novel metal-catalyzed enantioselective transfer hydrodeuteration method.