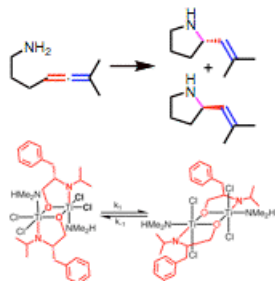


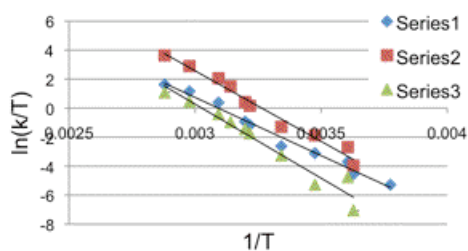
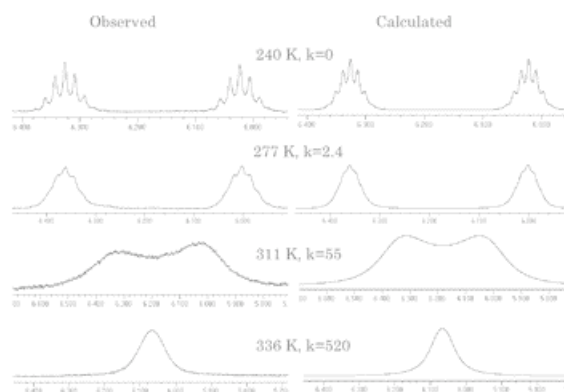
SYNTHESIS AND CHARACTERIZATION OF TITANIUM AMIDE ALKOXIDE COMPLEXES WITH DYNAMIC NMR BEHAVIOR

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Hydroamination is the addition of a nitrogen-hydrogen bond across a carbon-carbon double or triple bond. This reaction does not take place in a reasonable amount of time without a catalyst. In our case we use a titanium catalyst and a substrate that leads to a chiral product. By changing the ligand on the titanium catalyst we hope to form one enantiomer over the other.

The titanium catalyst exhibits fluxional behavior that can be characterized by nuclear magnetic resonance spectroscopy (NMR). By changing the temperature that the spectrum is taken we see both conformations at a low temperature and an average of the two at a higher temperature. The rate of change can be measured by modeling the spectra on a computer.



$$\ln \frac{k}{T} = -\frac{\Delta H^\ddagger}{R} \cdot \frac{1}{T} + \ln \frac{k_B}{h} + \frac{\Delta S^\ddagger}{R}$$

The rates were then fit to the Eyring equation to find the transition state entropy and enthalpy. Our hope is that knowing these values will give insight into the transition state of the conformational change. We can conclude that entropy and enthalpy are positive. Based on previous work this suggests that a large rearrangement occurs at the transition state. More work is needed to confirm this theory.

	<u>Series 1</u>	<u>Series 2</u>	<u>Series 3</u>
	d6 gNMR	d6 winDNMR	h gNMR
ΔH (kcal/mol)	15.9	19.3	20.3
ΔS (cal)	2.1	15.9	14.3



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