Department of Chemistry

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Mechanism of Halocarbene Additions to Cyclooctyne

Cyclooctyne (**1**) was successfully synthesized and purified from *cis*-cyclooctene (**10**) via 1-bromocyclooctene (**12**) in a 49% yield. This separation was incomplete, leaving residual **12**. Cyclooctyne (**1**) was in turn reacted with dibromocarbene. The suspected product of the carbene addition was isolated in order to identify it and thus determine the mechanism of its formation. GC/MS and ^{1}H, ^{13}C, DEPT-135, HSQC, and HMBC NMR spectra were used to try to characterize the product, with the results indicating that the carbene added selectively to **12** rather than **1**. Control reactions were run, reacting pure **12** with dibromo- and dichlorocarbenes, confirming that the originally isolated product was the result of carbene addition to **12**. Laser flash photolysis was used to measure the nanosecond kinetics of dichlorocarbene addition to **12**. This rate constant was found to be $k = 1.34 \times 10^{8}\ M^{-1}s^{-1}$. Future work will include determination of the rate constant for dichlorocarbene addition to **1** as well as the reaction of dihalocarbenes to very pure **1**.