

ABSTRACT

THESIS: The Kinetics of 1,3-Dipolar Cycloadditions of Azidopyridine *N*-Oxides

STUDENT: Breanna Ricketts

DEGREE: Master of Science

COLLEGE: Sciences and Humanities

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1,3-dipolar cycloaddition reactions of aromatic azides and alkenes or alkynes to form triazole and triazolines is a well established reaction. Reaction rate studies for phenyl azide with a variety of dipolarophiles have been previously performed by Huisgen, and then the reactivity and selectivity of those reactions were later explained by Sustmann in FMO terms. However, Sustmann did not use the entire set of reaction rates, since not all the FMO data were known at the time.

The first half of this thesis employed the use of computational chemistry to determine Frontier Molecular Orbital energies of the to determine the complete set of Huisgen and to generate a complete and updated FMO correlation diagram for phenyl azide cycloadditions, to determine the applicability of the Sustmann model for a broader range of dipolarophiles. The second half of this thesis was to experimentally determine the reaction rates of 1,3-dipolar cycloaddition reactions with azidopyridine *N*-oxides and a wide range of dipolarophiles in order to determine the role that the *N*-oxide group plays with respect to the reactivity and selectivity in 1,3-dipolar cycloaddition reactions of the azide moiety. In addition, these azidopyridine 1-oxides were observed to undergo tandem cycloaddition that is not seen with phenyl azide.