

SLATT UNDERGRADUATE RESEARCH FELLOWSHIP FINAL REPORT

SCHOLAR NAME:	Reinhard Bartsch
FACULTY ADVISOR:	Vlad Iluc
PROJECT PERIOD:	August 2022-Ongoing
PROJECT TITLE:	Isolation of Metallocyclobutane Intermediate for Ruthenium Catalyzed Olefin Metathesis as a Means of Bringing About More Sustainable Synthesis
CONNECTION TO ONE OR MORE ENERGY-RELATED RESEARCH AREAS (CHECK ALL THAT APPLY):	<input checked="" type="checkbox"/> Energy Conversion and Efficiency <input type="checkbox"/> Sustainable and Secure Nuclear <input type="checkbox"/> Smart Storage and Distribution <input type="checkbox"/> Transformation Solar <input type="checkbox"/> Sustainable Bio/Fossil Fuels <input type="checkbox"/> Transformative Wind

MAJOR GOALS AND ACCOMPLISHMENTS

Summarize your research goals and provide a brief statement of your accomplishments (no more than 1-2 sentences). Indicate whether you were able to accomplish your goals by estimating the percentage completed for each one. Use the next page for your written report.

RESEARCH GOALS	ACTUAL PERFORMANCE AND ACCOMPLISHMENTS	% OF GOAL COMPLETED
Synthesize PC(sp²)PRu Carbene in good yield	A new series of PC(sp ²)PRuCl ₂ L carbenes were synthesized and characterized.	100
Synthesize a Ru Carbene Analogous to the Iluc group's Fe carbene	A PC(sp ²)PRuL ₂ , L=PMe ₃ carbene was observed via NMR, only one labile ligand different from the current PC(sp ²)PFeL ₂ , L=PMe ₃ , N ₂ iron carbene.	80
Observe the formation of a Ru metallocyclobutane	Some reactivity has been observed between olefins and various modified Ru carbenes.	20

RESEARCH OUTPUT

Please provide any output that may have resulted from your research project. You may leave any and all categories blank or check with your faculty advisor if you are unsure how to respond.

CATEGORY	INFORMATION
EXTERNAL PROPOSALS SUBMITTED	(Sponsor, Project Title, PIs, Submission Date, Proposal Amount)
EXTERNAL AWARDS RECEIVED	(Sponsor, Project Title, PIs, Award Date, Award Amount)
JOURNAL ARTICLES IN PROCESS OR PUBLISHED	(Journal Name, Title, Authors, Submission Date, Publication Date, Volume #, Page #s)
BOOKS AND CHAPTERS RELATED TO YOUR RESEARCH	(Book Title, Chapter Title, Authors, Submission Date, Publication Date, Volume #, Page #s)
PUBLIC PRESENTATIONS YOU MADE ABOUT YOUR RESEARCH	(Event, Presentation Title, Presentation Date, Location) Notre Dame Summer Undergraduate Research Symposium
AWARDS OR RECOGNITIONS YOU RECEIVED FOR YOUR RESEARCH PROJECT	(Purpose, Title, Date Received)
INTERNAL COLLABORATIONS FOSTERED	(Name, Organization, Purpose of Affiliation, and Frequency of Interactions)
EXTERNAL COLLABORATIONS FOSTERED	(Name, Organization, Purpose of Affiliation, and Frequency of Interactions)
WEBSITE(S) FEATURING RESEARCH PROJECT	(URL)
OTHER PRODUCTS AND SERVICES (e.g., media reports, databases, software, models, curricula, instruments, education programs, outreach for ND Energy and other groups)	(Please describe each item in detail)

RESEARCH EXPERIENCE

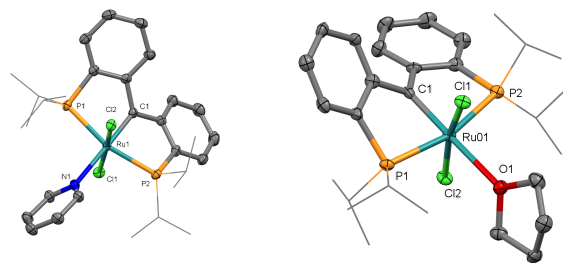
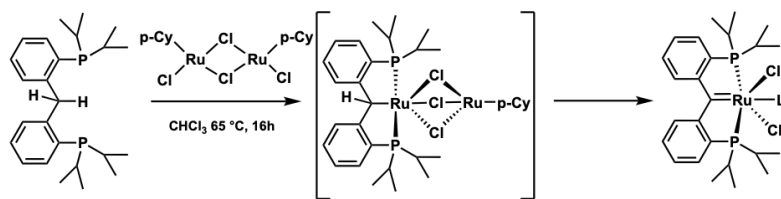
Please let us know what you thought of your research experience: Did this experience meet your expectations? Were lab personnel helpful and responsive to your needs? What else could have been done to improve your experience or achieve additional results?

This experience was extremely useful for me because I learned what it was like to work full-time in a laboratory, as one does in graduate school. This helped guide my decision in choosing to attend graduate school and work towards a PhD in chemistry after I graduate from Notre Dame. Lab personnel were helpful teaching me specific laboratory procedures, sharing reagents, and assisting with project development over the course of my time this summer. The only thing I wish I had more of to achieve additional results is: time. I will remain with the same lab during the school year to continue my project.

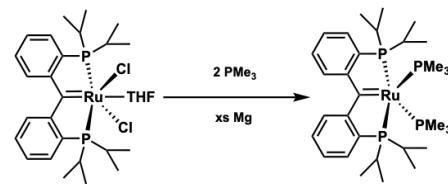
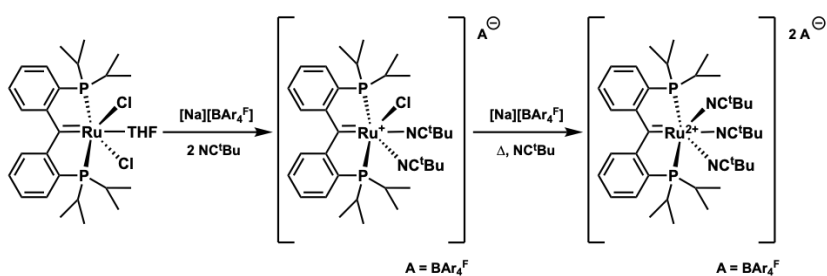
FINAL WRITTEN REPORT

(Please use the space below to describe your research project and objectives, any findings and results you can share, and graphs, charts, and other visuals to help us understand what you achieved as a result of this research experience.)

The Iluc group works on isolating reactive species intermediates, largely for catalytic cycles. My research goal is to isolate a metathesis active metallocyclobutane on ruthenium. This is essential because it provides key insight into the mechanism at work in olefin metathesis. This would contribute to the field of synthetic organic chemistry by assisting other groups working with metathesis in their catalyst design process and rate modifications. Furthermore, by performing metathesis with the PCP ligand on ruthenium, I can contribute to the Iluc group's iron catalyzed olefin metathesis project that uses the same PCP ligand. This would be beneficial since iron is a far more abundant element which would bring about more sustainable synthetic methods for chemistry. From August 2022 until June 2023 I was working on synthesizing a ruthenium carbene with consistent yield. By June, I was able to produce various $PC(sp^2)PRuCl_2L$ carbenes with consistently high yield. I collected crystal structures of two carbenes from this series, (L = THF, py).



After completing this stage of my research, I was able to move on testing the reactivity of my carbenes. As expected, the lack of open coordination sites on the metal center, *cis* to the carbene, prevented this series of ruthenium carbenes from exhibiting reactivity with olefins (styrene, norbornene) and alkynes, (diphenylacetylene). I spent the rest of the summer synthesizing various modified carbenes with greater expected reactivity. I tried many combinations of reductants and more labile ligands in order to synthesize a reduced carbene. I was able to synthesize a $PC(sp^2)PRuL_2$, L=PMe₃ carbene (by NMR). This Ru(II) carbene's expected trigonal bipyramidal geometry could allow an olefin to approach the carbene for metathesis to occur. Additionally, I was able to synthesize a monocationic and a dicationic carbene with pivalonitrile ligands. I collected crystal structures of both of these carbenes as well.



I am yet to test the reactivity of the newly characterized cationic carbenes. I will heat both carbenes in the presence of olefins and alkynes in hopes of achieving reactivity. Furthermore, I intend to continue pursuing different reductant and ligand combinations in the hopes of producing different reduced carbenes.

Future Directions

