SLATT UNDERGRADUATE STUDENT FELLOWSHIP

CHECK ONE: [ ] UPDATE [x] FINAL REPORT

SLATT SCHOLAR:	Anthony Deziel
FACULTY ADVISOR:	Professor Vlad Iluc
REPORT PERIOD:	Fall 2018 – Spring 2019
PROJECT TITLE:	Square Planar Nucleophilic and Radical Pt(II) Carbenes
CONNECTION TO ND ENERGY'S RESEARCH AREAS (CHECK ALL THAT APPLY):	**(X) Energy Conversion and Efficiency ( ) Sustainable and Secure Nuclear ( ) Smart Storage and Distribution ( ) Transformation Solar ( ) Sustainable Bio/Fossil Fuels ( ) Transformative Wind**

MAJOR GOALS AND ACCOMPLISHMENTS:

List your major research goals and provide a brief description of your accomplishments (1-2 sentences). Indicate the percentage completed for each goal. Please use a separate sheet to share additional details, technical results, charts, and graphics.

MAJOR RESEARCH GOALS	ACTUAL PERFORMANCE AND ACCOMPLISHMENTS	% OF GOAL COMPLETED
Publish a peer reviewed paper	I was able to successfully publish a first author paper in a peer reviewed journal.	100
Fully characterize all carbenes	All of the carbenes synthesized had characterization by H NMR and P NMR, elemental analysis, XRD crystallography. Due to insolubility, one carbene could not be characterized via C NMR and Pt NMR, but the other carbene was.	90
Fully characterize all precursors	All precursors were fully characterized by H, C, P, Pt NMR, XRD crystallography and elemental analysis.	100
Discover new reactivity of the carbenes	The reactivity of the new carbenes has only been probed. They have been shown to react with small molecules (HCl, H2O), had their thermal instability determined to be 140 C, been oxidized to radicals, and have been reacted with silanes (SiH2(Ph3)2) and (SiH(Ph3)3). However, there are many future reactions (such as germanes) that have yet to be studied. Many products have yet to be fully characterized.	35
Discover new reactivity of the radical carbene species	The radical carbenes are fully characterized via Evans method, EPR, and XRD crystallography. Further oxidation may be possible with NaBarF but remains untested.	50
Learn how to communicate my research in oral, visual, and written forms	I have practiced my visual, oral, and written communication several times through various powerpoint presentations, meetings with visiting speakers, and poster presentations. However, I have yet to give a large lecture and these skills can always be improved. Preparation of a thesis and peer reviewed article have improved my writing skills.	75

RESEARCH OUTPUT:

Please provide detailed information below regarding any output resulting from your research project. Please check with your faculty advisor if you are unsure how to respond.

CATEGORY	INFORMATION
EXTERNAL PROPOSALS	(Sponsor, Project Title, PIs, Submission Date, Proposal Amount)
EXTERNAL AWARDS	(Sponsor, Project Title, PIs, Award Date, Award Amount)
JOURNAL ARTICLES	(Journal Name, Title, Authors, Submission Date, Publication Date, Volume #, Page #s) **Journal: Organometallics, Title: Square Planar Nucleophilic and Radical Pt(II) Carbenes, Authors: Anthony P. Deziel, Melissa R. Hoffbauer, Vlad M. luc, Submitted 11/29/18, Published 2/15/19, Vol 38, Issue 4, Pages 879-887**
BOOKS AND CHAPTERS	(Book Title, Chapter Title, Authors, Submission Date, Publication Date, Volume #, Page #s)
PUBLIC PRESENTATIONS, SEMINARS, LECTURES	(Event, Presentation Title, Presentation Date, Location) **COS-FURF, Synthesis Characterization and Oxidation of a Platinum(II) Carbene, 10/25/18, Notre Dame**

	PINDU Inorganic Symposium, Square Planar Nucleophilic and Radical Pt(II) Carbenes, 12/1/18, Notre Dame
AWARDS, PRIZES, RECOGNITIONS	(Purpose, Title, Date Received) **PINDU Inorganic Symposium Best Undergraduate Research Poster – 12/1/28** **Outstanding Chemist Award – 5/3/19**
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) **Honors Chemistry Thesis – This project provided a portion of the research which was included in my Honors Chemistry Thesis for the Undergraduate Honors Chemistry program at Notre Dame.**

RESEARCH EXPERIENCE:

Please let us know what you thought of your research experience: Did this experience meet your expectations? Was there something else that could have been done to improve your research experience? Were lab personnel helpful and responsive to your needs? What could have been done differently, if anything, to achieve additional research results?

I very much enjoyed this research experience. It was fulfilling to achieve the goals which I had set out for myself, including the publication of a research paper. Being able to contribute to the world of science in a meaningful way has been a highlight of this research experience. Additionally, I believe that this research experience has thoroughly prepared myself to be a successful graduate student pursuing my PhD at Yale in the fall. The lab personnel were extremely helpful. Dr. Ian Lightcap from the MCF was always available to help with the instruments in the facility and Dr. Allen Oliver was very helpful in the Xray Crystallography lab. My graduate student mentor, Melissa Hoffbauer, has been amazing to work with and helped me throughout the entire project. One minor improvement to the research experience could be additional funding for conference travel. Attending the ACS conference would be exciting, though it is often far away and expensive. In terms of results, I did not feel restricted by the facilities or funding, just by my own experience and time.

MAJOR GOALS AND ACCOMPLISHMENTS
(Additional Details, Technical Results, Charts and Graphics)

I was unable to obtain a ^{13}C NMR for the first platinum carbene which I had synthesized due to the insolubility of the platinum carbene complex. This prompted the synthesis of an addition platinum carbene on a new ligand containing a functional group substitution on the benzene rings. The ^{t}Bu functional group increased solubility and allowed for the observation of the carbene carbon peak in the ^{13}C NMR spectrum. This peak is shown in Figure 1.

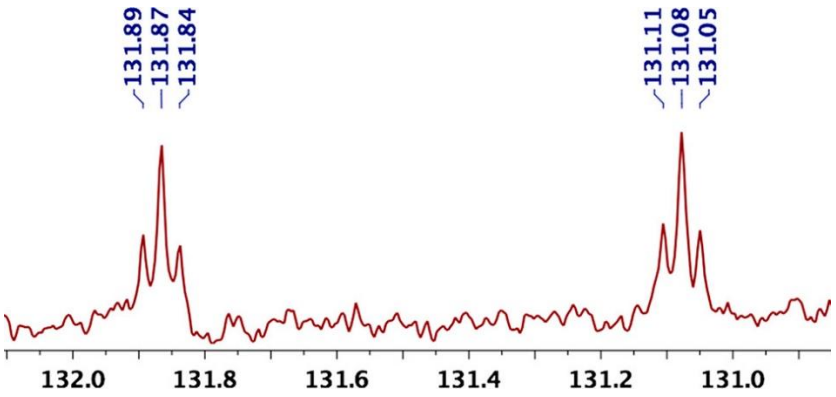

Figure 1. 13C NMR of the carbene carbon region for the platinum carbene, $[PCP]^{tBu}PtPMe_3$.

XRD crystallography revealed the solid state structure of the platinum carbenes and platinum carbene radical. These structures can be seen in Figures 2-4.

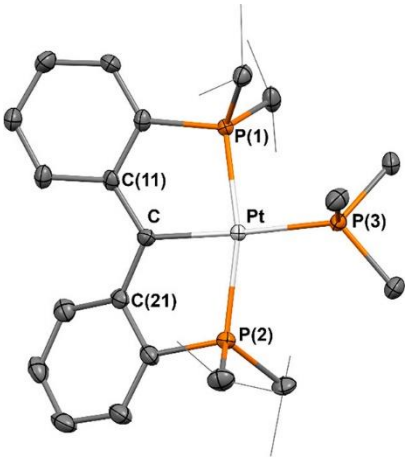

Figure 2. Solid state structure of $[PCP]^{H}PtPMe_3$ from single crystal XRD crystallography studies.

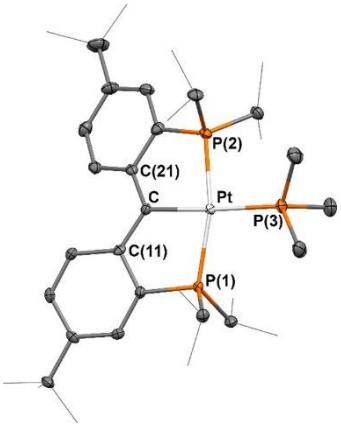

Figure 3. Solid state structure of $[PCP]^{tBu}PtPMe_3$ from single crystal XRD crystallography studies.

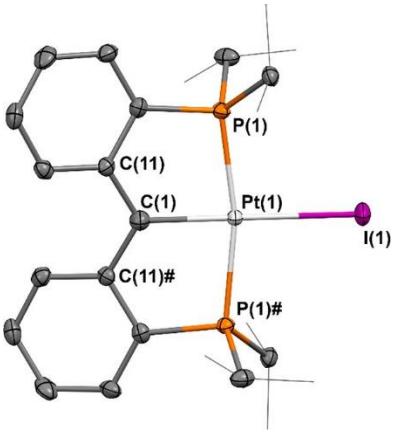

Figure 4. Solid state structure of $[PC^{\cdot}P]^{H}PtPMe_3$ from single crystal XRD crystallography studies.

Additional characterization of the platinum carbene radical can be seen in Figure 5. This characterization was necessary due to the paramagnetic nature of the radical, where NMR studies were silent.

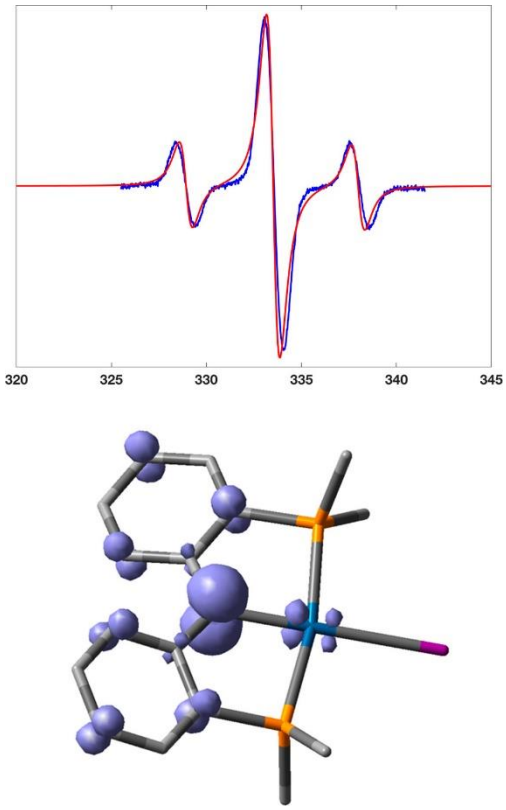

Figure 5. EPR and Spin Density Calculations of the Platinum Carbene Radical, $[PC^{\cdot}P]^{H}PtPMe_3$