# Using Animations to Visualize Olefin Metathesis Chemical Reactions

Savannah Hall and Janet Coonce


## ABSTRACT

A series of animations and PowerPoint presentations have been created to help introductory chemistry students visualize the Chauvin mechanism for olefin metathesis chemical reactions. Olefin metathesis is the subject of the 2005 Nobel Prize for chemistry, and the reaction can be difficult to describe with static diagrams. For this reason, a team of high school and undergraduate chemistry students at Tennessee Technological University have created animations of olefin metathesis reactions to demonstrate how the atoms rearrange in the chemical reaction. The reaction animations are available with open-access for presenters to download editable files.


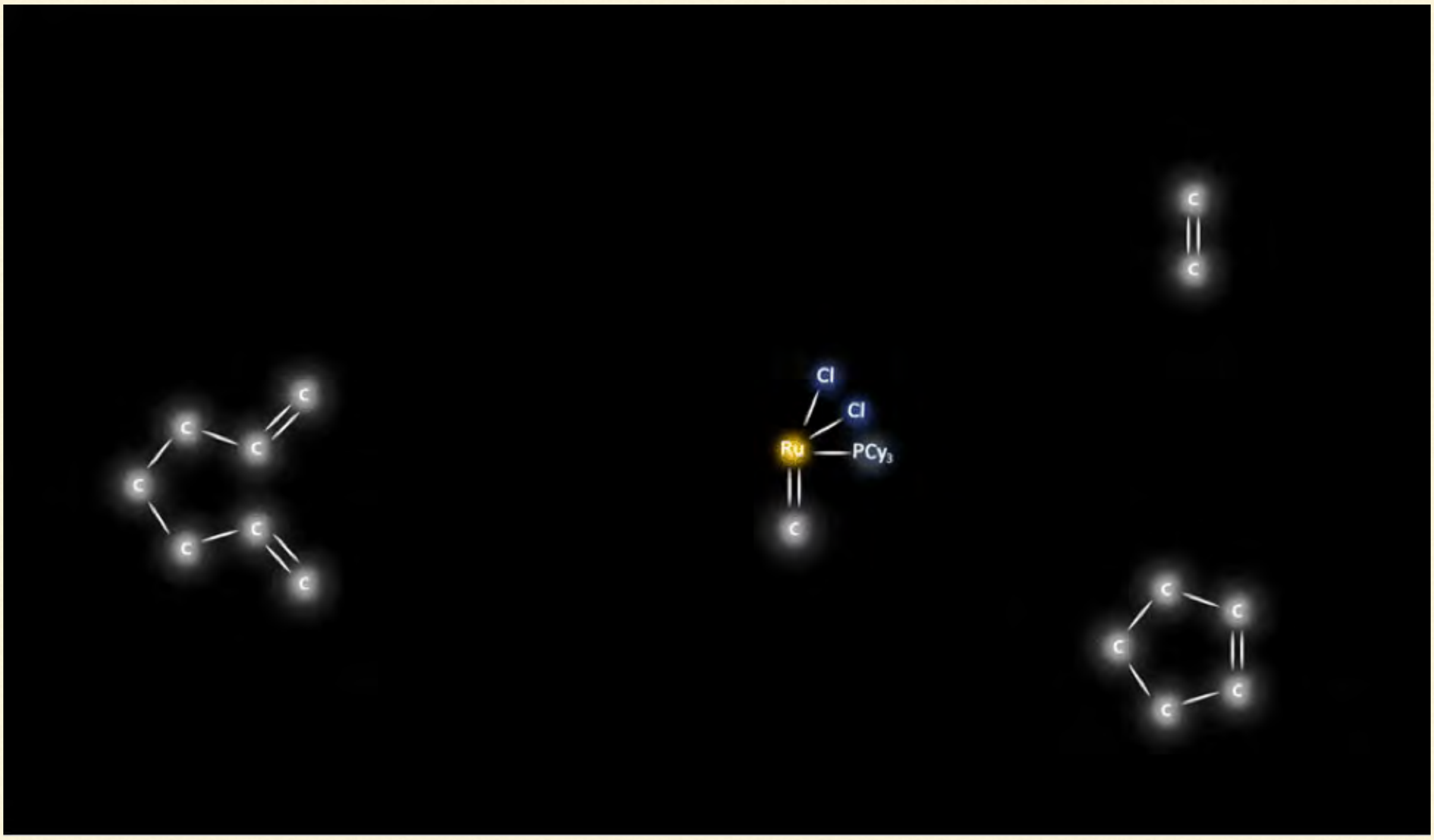


*Figure 1. Animated .gif file of the catalytic cycle of the Ring Closing Metathesis (RCM) mechanism using Grubb's 1st generation ruthenium catalyst. Savannah Hall, 2017.*

## Introduction

The olefin metathesis chemical reaction has been studied extensively over the past forty years, and it is one of the most widely-used chemical reactions in industry and academics today.(1) An olefin is simply a compound that contains at least one carbon-carbon double bond, and another term for an olefin is an alkene. In an olefin metathesis reaction, one carbon of a carbon-carbon double bond changes places with another carbon of a second carbon-carbon double bond to form two new carbon-carbon double bonds.(2) The olefin metathesis reaction allows chemists to make new organic compounds including medicines, plastics, and other petroleum products that were previously slow, difficult, or unable to be synthesized.(3)

In 1971, French chemist Yves Chauvin explained the mechanism for how the atoms might rearrange in the metal-catalyzed olefin metathesis reactions.(4) Since then, new olefin metathesis catalysts and uses for the olefin metathesis reaction have been discovered and developed. Notably, Richard R. Schrock and his research group at Massachusetts Institute of Technology (MIT) have continued to produce efficient metal catalysts for metathesis using molybdenum ($Mo^{6+}$), tungsten ($W^{6+}$), and other metal centers.(5) Robert H. Grubbs and his research group at California Institute of Technology (CalTech) have continued to develop air-stable catalysts using ruthe-nium ($Ru^{2+}$) and other metal centers.(6) In 2005, the Nobel prize for chemistry was awarded jointly to Chauvin, Grubbs, and Schrock "for the development of the metathesis method in organic synthe-sis."(7)

## Chauvin Mechanism

The Chauvin mechanism is the currently-accepted mechanism for the olefin metathesis reaction. This mechanism has been described as, "a pair-wise interchange of carbon atoms."(8) Figure 2 displays an example of the written Chauvin mechanism applied to a ring-closing metathesis (RCM) reaction of 1,6-heptadiene to form cyclopentene in the presence of a 1st Generation Grubb's catalyst. Unfortunately, written mechanisms such as these can be quite difficult for introductory chemistry students to initially visualize, especially without the necessary background knowledge or professional guidance. The goal of this creative inquiry project is to make simple animations of metathesis mechanisms in an easily-accessible format for students, presenters, and educators alike.

## Animation and Powerpoint Progression

This project first began in the summer of 2014 when Tennessee Tech's Governor's School for Emerging Technology created simplified animations of (1) cross metathesis (CM), (2) Ring Closing Metathesis (RMC), (3) Ring Opening Metathesis (ROM), (4) Ring Opening Metathesis Polymerization (ROMP), (5) Acyclic Diene Metathesis (ADMET), and (6) Ethenolysis. Eight high school-level students worked in teams of two and three to research how these reaction worked, and then they explored Adobe Edge Animate to create scalable HTML5 web-based animations to help web viewers visualize the mechanism of the catalytic cycle of each metathesis reaction. These animations can be viewed at:
https://animations.connectingchemistry.com/TNgovschool/

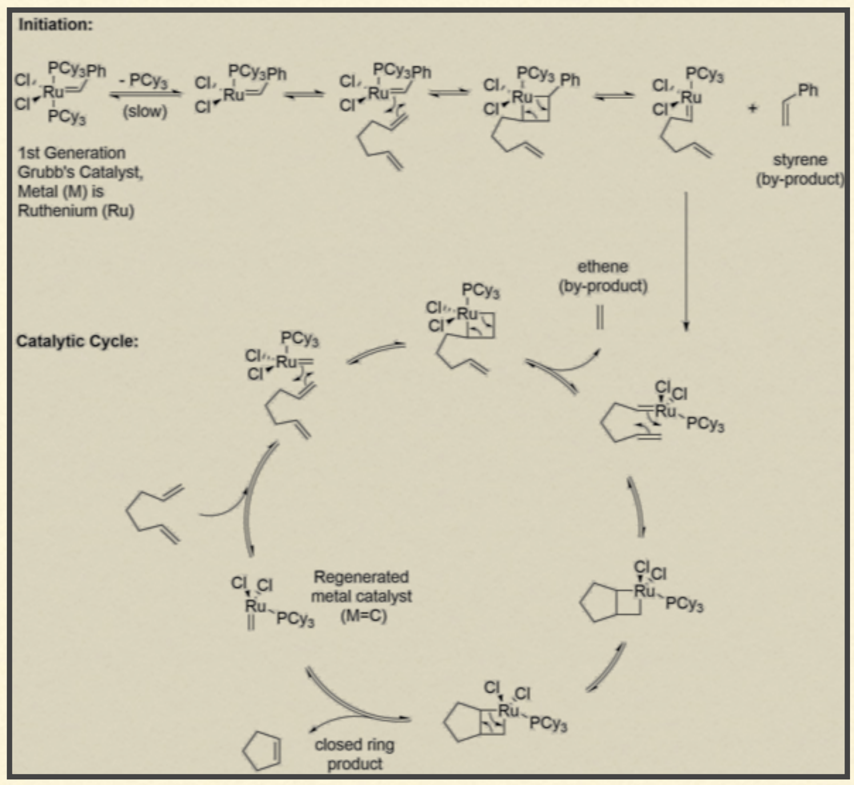


*Figure 2. Chauvin mechanism of a simple Ring-Closing Metathesis (RCM) reaction, showing both the initiation and the catalytic cycle.(2,10)*

After the Governor's School students published their animations online, the next step was to make the animations more accessible to educators who wished to use them offline. The animations were converted to animated .gif files and recreated for use in PowerPoint slides. The Governor's School animations depicted the metathesis catalyst (M=C) as a generic and simple metal-centered catalyst double-bonded to a carbon, without specifying ligands and alkyl groups. In the next set of animations, the generic gold-colored metal center (M) of the catalyst in the Governor's school student animations was specified as ruthenium (Ru) in the 1st Generation Grubb's Catalyst (Figure 3).

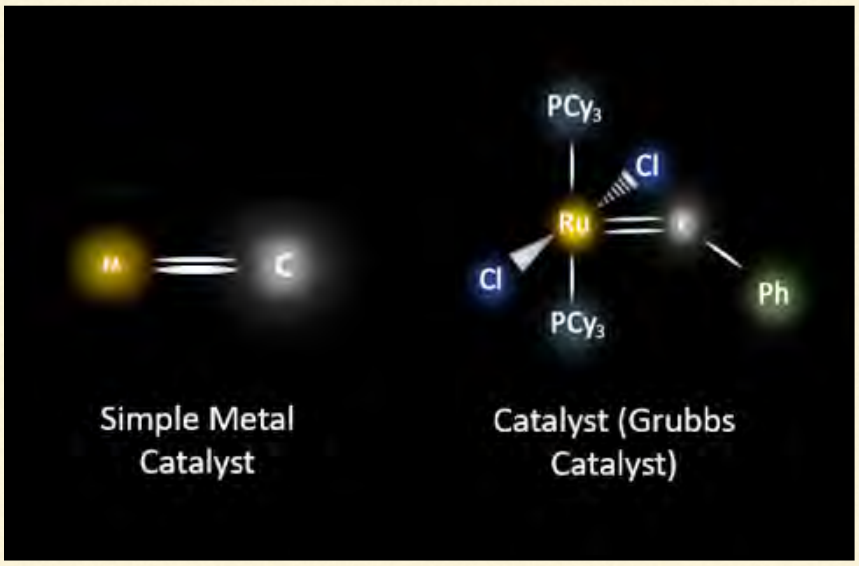


*Figure 3. Comparison of initial metal catalyst used by the Governor's School students to the original first generation Grubb's Catalyst. PowerPoint slide by Savannah Hall, 2017.*

Choosing to designate a specific Grubb's catalyst allowed us to animate the initiation step required to activate the catalyst. We were able to show the removal of a tricyclohexylphosphine ($PCy_3$) group and explain the minor product, styrene, $CH_2CHPh$ (shown highlighted with a green Ph) in the animation. Even though much more effective catalysts [9] have been developed since the development of the 1st Generation Grubb's catalyst, this catalyst was chosen for simplicity's sake in order to demonstrate the mechanism of both the initiation and catalytic cycle. The new animated files were created to display the complete mechanism for the specific reaction of 1,6-heptadiene to form cyclopentene in the presence of a 1st Generation Grubb's catalyst (Figure 4).

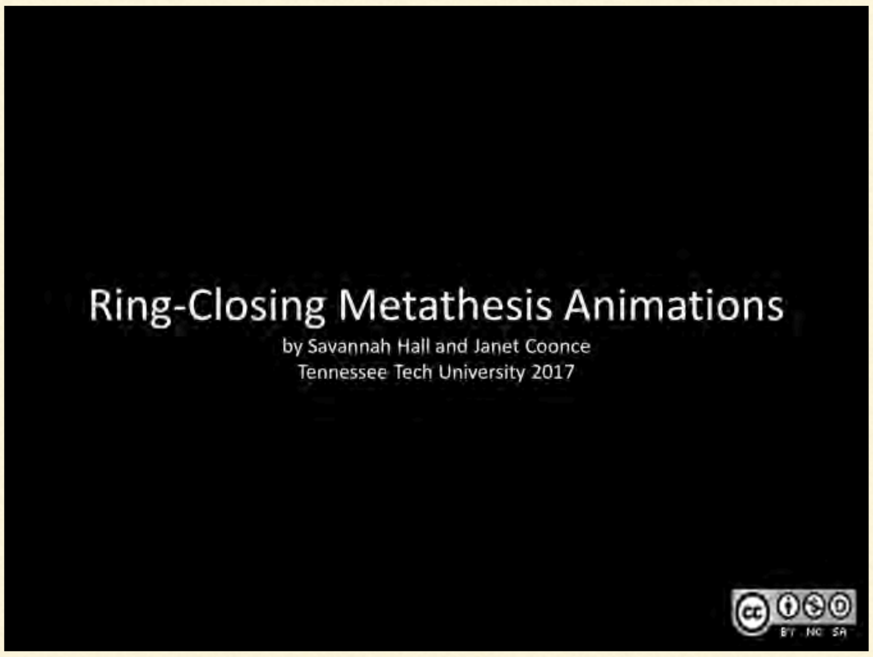


*Figure 4. Initiation and catalytic cycle of the Chauvin mechanism for the ring closing metathesis reaction. Savannah Hall, 2017.*

The new PowerPoint slides were used as rough draft precursors to developing a more fluid animation in Adobe Edge Animate for scalable HTML5 web browser viewing. Animations were made for both Ring-Opening and Ring-Closing Metathesis reactions, each having a version where the phenyl removal step was included (showing the initiation step and the catalytic cycle) and one where it was not (showing only the repeating catalytic cycle). However, using Adobe Edge to publish to the internet can be difficult if one is not familiar with HTML or JavaScript coding. These animations also need live internet access to show in a presentation. A solution to this problem was to turn the Edge file into a GIF file that could be easily downloaded and viewed in a presentation by using the recording software Camtasia Relay and Adobe Photoshop.

Each metathesis animation was recorded using Camtasia, and then Adobe Photoshop was used to export the video to a hi-definition GIF. The main advantages to using animated GIF files is that they can be easily shared and viewed in PowerPoint without internet access. The disadvantage is that the GIF files cannot be paused for discussion. To overcome this disadvantage, the animations can be viewed either as a step-by-step PowerPoint animation or as a more-fluid and powerful HTML5 animation file online at: https://animations.connectingchemistry.com/TTU/.

**Conclusion**

All metathesis animations, GIFs, and PowerPoint slides were successfully created, and they are available for all students, presenters, and educators to freely downloaded and modify. The intent of these animations is that they could be used in discussions in any language, and at many different levels of chemical understanding. All work is licensed under a Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International License. This means all non-commercial parties may use, remix, transform, or build upon the material and freely distribute contributions with the attribution, "Savannah Hall and Janet Coonce, Tennessee Tech University, Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International License © 2017." Our hope is that some or all of these animations will be useful to both students and presenters. Future work includes the animation of additional chemical reaction mechanisms.

**Acknowledgements**

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