Chemistry 145 – Spring 2021

Inorganic and Organometallic Chemistry with Laboratory

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* **Point distribution**

|  |  |
| --- | --- |
| Written assignment – 1st draft | 20 points |
| Written assignment – final draft | 36 points |
| Presentation slide deck – 1st draft | 20 points |
| Presentation slide deck – final draft | 35 points |
| Oral presentation | 39 points |
| Total | 150 points |

* **Schedule**

|  |  |
| --- | --- |
| Submit [survey](https://forms.gle/FKaum93fsSH1PZ8RA) of topic choice | Jan 29th |
| Topic and presentation date posted | Feb 5th |
| Written assignment – 1st draft | March 12th |
| Written assignment – final draft | April 2nd |
| Presentation slide deck – 1st draft | April 23rd |
| Presentation slide deck – final draft | Day of presentation |
| Oral presentation | May 3rd, May 5th |

* **Project overview**

In this project, you will practice using green chemistry principles and systems thinking to become familiarized with a specific area of coordination chemistry and organometallic research. You will be given a paper as a starting point to conduct further research into the importance of the field. There is a written portion and a presentation portion to this project, totaling 150 points. You must submit a survey (<https://forms.gle/FKaum93fsSH1PZ8RA>) ranking your choice of topics (found at the end of this guide) by Jan 29th. Your topic will be assigned on Feb 5th.

As industry progresses, the pollution to Earth also becomes more severe. Modern chemists use the 12 principles of green chemistry (<https://www.epa.gov/greenchemistry/basics-green-chemistry>) to guide the design of new reactions and improve on old reactions. These principles focus on minimizing the impact of chemical industrial activities on our environment while maintaining the production of important consumer products that improve the quality of life around the globe.

When you study your paper(s), you want to focus on these green chemistry principles and think about how every design detail of a chemical reaction or process can impact our lives in these contexts.

* **Written assignment**

Each student will submit a 1.5 to 2-page introduction (references not included) to your paper and the topic it explores. Your written assignment must include a detailed list of references in ACS style (see style guide posted on Canvas). You may have a maximum of two graphs or tables and each must be accompanied with a detailed description.

The 1st draft will be peer-reviewed in class and the grade will be based on the average of the scores assigned by your classmates using the rubric given at the end of this document. The final draft will be graded by the instructor.

Use the following questions to guide you.

1. Why is this topic of interest to scientists?

Is there a specific target product and how is the product important to society?

If there is not a specific product, is there a specific functional group that they are aiming to transform and how is the reaction important to society?

1. How is the target product currently being produced? or How is the functional group transformation currently performed?
2. Is the current production method sustainable?

Are there unsustainable starting materials?

Are there unsustainable reagents/catalysts?

Are there toxic byproducts?

Are there dangerous procedures involved?

1. What are the authors in the paper proposing to improve on the current production method?

Choose more sustainable starting materials?

Choose more sustainable or higher activity reagents and catalysts?

Design a reaction that produces less by products?

Design a safer reaction?

* **Presentation**

The presentation should be 30-mins in length. Your presentation must be accompanied by a slide deck in Powerpoint or similar applications. The 1st draft of your slide deck will be peer-reviewed in class and the grade will be based on the average of the scores assigned by your classmates using the rubric given at the end of this document. The final draft of your slide deck will be due on the day of your presentation and will be graded by the instructor. You will also receive a score for the oral presentation that you give.

Generally, a presentation begins with an introduction to the topic so your presentation should build on your written assignment (which you wrote as an introduction to the paper). The most important additional elements in your presentation a detailed description of the chemistry behind the authors’ work and the conclusions. Use the following questions to guide your preparation.

1. An introduction to the topic. This is covered in your written assignment.
2. Background chemistry of the proposed work. Generally, you will find this information in the references cited in the paper.
   1. Why was the specific ligand chosen?
   2. Why was the specific metal chosen?
   3. What were the difficulties exhibited in previous works when researchers attempted the same or similar reactions?
   4. What previous observations or literature convinced the authors that their new idea would work better?
3. Description of the work.
   1. How was the catalyst synthesized?
   2. What important reagents were used and what were the roles of the reagents?
   3. How was the reaction conducted? Temperature, time, solvent, pressure……etc.
   4. Discussion of the results. Turnover number, turnover frequency, product selectivity, product yield…… etc.
   5. What is the proposed mechanism? What analytical techniques were employed to investigate the mechanism?
   6. If some steps in the proposed mechanism are vague, can you make further hypotheses using what you have learned in class?
4. Conclusion.
   1. What were the improvements made by the authors compared to current applied methods?
   2. What were the improvements made by the authors compared to other researchers in the field?
   3. What are the lasting impacts of this work? Can it spur further research or does it indicate that this is a dead end?
   4. Personal comments?

* **Rubrics**

Written assignment:

|  |  |  |
| --- | --- | --- |
|  | 1st draft | Final draft |
| **Style** |  |  |
| Organization | **/2** | **/3** |
| Clarity of language | **/2** | **/3** |
| Sufficient references | **/2** | **/3** |
| Figures and tables used appropriately | **/2** | **/3** |
| **Content** |  |  |
| Importance of the reaction | **/4** | **/8** |
| Drawbacks of current methods | **/4** | **/8** |
| Improvements made in the paper | **/4** | **/8** |
| Total | **/20** | **/36** |

Powerpoint:

|  |  |  |
| --- | --- | --- |
|  | 1st draft | Final draft |
| **Style** |  |  |
| Organization and clarity | **/2** | **/3.5** |
| References cited appropriately | **/2** | **/3.5** |
| Figures and tables used appropriately | **/2** | **/3.5** |
| **Content** |  |  |
| Introduction | **/2** | **/3.5** |
| Background | **/2** | **/3.5** |
| Description of catalysts and reagents | **/2** | **/3.5** |
| Description of reaction | **/2** | **/3.5** |
| Discussion of the results | **/2** | **/3.5** |
| Proposed mechanism | **/2** | **/3.5** |
| Conclusion | **/2** | **/3.5** |
| Total | **/20** | **/35** |

Presentation

|  |  |
| --- | --- |
|  | Presentation |
| **Style** |  |
| Voice projection and tone | **/2** |
| Speed and clarity | **/2** |
| **Content** |  |
| Clarity of explanations | **/5** |
| Defining terms/jargon | **/5** |
| Understanding of the background | **/5** |
| Understanding of the reagents | **/5** |
| Understanding of the mechanism | **/5** |
| Fully grasp the conclusion and impacts | **/5** |
| Handling questions | **/5** |
| Total | **/39** |

* **Topics and papers**

Ammonia production: metal-catalyzed nitrogen hydrogenation

<https://www.nature.com/articles/ncomms4737>

Formic acid synthesis: carbon dioxide hydrogenation

<https://www.nature.com/articles/ncomms5017>

Alcohol oxidation: metal catalyzed acceptorless dehydrogenation

<https://pubs.acs.org/doi/10.1021/ja210857z>

Olefin hydrosilylation: base-metal catalysis

<https://science.sciencemag.org/content/335/6068/567>

Reduction of carboxylic acid derivatives: metal-catalyzed hydrogenation

<https://science.sciencemag.org/content/350/6258/298.full?ijkey=lOqLMtmIodP.A&keytype=ref&siteid=sci>

**Green chemistry's 12 principles**

These principles demonstrate the breadth of the concept of green chemistry:

**1. Prevent waste**: Design chemical syntheses to prevent waste. Leave no waste to treat or clean up.

**2. Maximize atom economy**: Design syntheses so that the final product contains the maximum proportion of the starting materials. Waste few or no atoms.

**3. Design less hazardous chemical syntheses**: Design syntheses to use and generate substances with little or no toxicity to either humans or the environment.

**4. Design safer chemicals and products**: Design chemical products that are fully effective yet have little or no toxicity.

**5. Use safer solvents and reaction conditions**: Avoid using solvents, separation agents, or other auxiliary chemicals. If you must use these chemicals, use safer ones.

**6. Increase energy efficiency**: Run chemical reactions at room temperature and pressure whenever possible.

**7. Use renewable feedstocks**: Use starting materials (also known as feedstocks) that are renewable rather than depletable. The source of renewable feedstocks is often agricultural products or the wastes of other processes; the source of depletable feedstocks is often fossil fuels (petroleum, natural gas, or coal) or mining operations.

**8. Avoid chemical derivatives**: Avoid using blocking or protecting groups or any temporary modifications if possible. Derivatives use additional reagents and generate waste.

**9. Use catalysts, not stoichiometric reagents**: Minimize waste by using catalytic reactions. Catalysts are effective in small amounts and can carry out a single reaction many times. They are preferable to stoichiometric reagents, which are used in excess and carry out a reaction only once.

**10. Design chemicals and products to degrade after use**: Design chemical products to break down to innocuous substances after use so that they do not accumulate in the environment.

**11. Analyze in real time to prevent pollution**: Include in-process, real-time monitoring and control during syntheses to minimize or eliminate the formation of byproducts.

**12. Minimize the potential for accidents**: Design chemicals and their physical forms (solid, liquid, or gas) to minimize the potential for chemical accidents including explosions, fires, and releases to the environment.