**Electronic Structure Report: Determination of Reaction Mechanism**

**Due date**: November 7, 2019

**This will be done in groups of 3-4, but everyone must turn in their own report.**

Two mechanisms have been proposed for the following dehydration reaction:



Mechanism 1:



Mechanism 2:



The group proposing the mechanisms suggests that the second scheme is unlikely because secondary alcohols dehydrate by an E1 mechanism and not an E2 mechanism. This is because water is not a strong base, which is required for an E2 mechanism.

**Goal:** The goal of this report will be to use electronic structure calculations to compare the thermodynamics of both mechanisms and determine which is the most likely in terms of thermodynamics.

**The central questions that your paper should answer are:**

1. What is the change in internal energy, enthalpy, free energy and entropy the overall reaction?
2. What is the change in internal energy, enthalpy, free energy and entropy for each step in the reaction?
3. Is the overall reaction driven by entropy or enthalpy?
4. Are the individual steps enthalpically or entropically driven?
5. What is the best mechanism based on thermodynamics.

**Remember: For thermochemistry, products minus reactants (all products, all reactants)**

**Other items you are free to consider (no guarantees)**

1. What role might the electrostatic potential play in the reaction?
2. How might the HOMO and LUMO orbitals explain the reactivity?
3. Do the normal modes of the molecule suggest the observed reactivity?

**Some bonus questions if you are ambitious**

1. What role does stereochemistry play in the reaction?
2. How does adding an electron withdrawing group near the alcohol affect the reaction?
3. How does adding an electron donating group near the alcohol affect the reaction?

**Format**

The format of this report should follow the guidelines of the *Journal of Chemical Theory and Computation*.

<https://pubs.acs.org/page/jctcce/submission/authors.html#TEMPLATES>

You should look at some papers from the journal to get a sense of how people write for it.

**The page limit is 5 pages**. If you need to show extra data, you can include it in a supplemental information section, the main paper and findings must be 5 pages.

**Grading Rubric**

This report should look like a real paper.

1. Title
2. Abstract
   1. an image for the abstract
3. Introduction
4. Computational Details (Methods)
5. Results and Discussion
6. Conclusion
7. Bibliography
   1. Note: You need to cite software that you use

All entries will be given grades from 0-4

**Format:**

4 – The JCTC format was followed, all required features are included, all figures all numbered. The paper looks clean and professional

3 – Minor issues

2 – Distracting issues, or something is missing

1 – Many issues, very distracting, missing sections

0 – Did not follow formatting

**Readability:**

4 – Easy to read, language is clear and understandable

3 – Minor grammatical issues but overall well written

2 – Issues with readability make argument hard to follow

1 – Many grammatical issues, sloppy writing

0 – Nearly unreadable

**Science and results:**

4 – Scientific argument is logical and clear. Answered all required questions and said something interesting about the reaction. You use your data to come to a “big picture” conclusion about chemistry.

3 – Scientific argument is logical and clear. Answered all required questions and said something interesting about the reaction.

2 – Some issues with your argument or logic. Answered all or most of required questions and said something interesting about the reaction.

1 – Flawed argument or logic. Issues with calculations. Missing some of the required questions

0 – No argument or context. Just a list of results.

**Figures and tables**

4 – Figures/tables support the argument, are numbered, are described in the text, have good descriptions that says something important about the figure, and look good.

3 – Figures/tables support the argument, are numbered, are described in the text. The figures look clean and professional

2 – Figures mostly support the argument, are numbered, and referred to in the text. The figures mostly look good, but there are some issues with resolution, coloring, etc.

1 – The figures either do not support the arguments, are not labeled correctly, are not referred to in the text, or have some other major presentation issues

0 – Why aren’t there figures?

**Title:**

2 – Title says something interesting about the study and is catchy

1 – A good enough title

0 – No title, or just recycled the title at the top of the page

**Abstract:**

2 – Abstract connects to big picture and is good enough to be cited without having to read the paper

1 – The abstract does a good enough job summarizing the paper

0 – Something is deeply wrong with the abstract, does not tell you about the paper.

**Introduction:**

3 – Describes chemistry background, big picture importance of system, and how using electronic structure will lead to a new understanding. A great job setting up the entire rest of the paper.

2 - Describes chemistry background and electronic structure background. Lacking some of the big picture.

1 – Introduction does not do a great job describing chemistry, or motivating the paper.

0 – Introduction missing, deeply flawed, or unrelated.

**Computational Methods:**

3 – It is clear what methods, models, and software were used to run the simulations. Justifications given for chosen methods. Anyone reading this would understand what was done and why.

2 – All methods, models, and software described. Justifications not always clear.

1 – Major information missing from methods.

0 – I can’t tell what you did

See this list to see how people write methods when using Gaussian:

<https://pubs.acs.org/doi/pdf/10.1021/ja8025906>

<https://gaussian.com/top25/>

How to cite Gaussian

<http://gaussian.com/citation/>

**Results/Discussion:**

3 – All data is described and placed into context. All figures help the argument and are referred to in the text. Discussion uses results to strengthen the argument and show “big picture”

2 - All data is described and placed into context. All figures help the argument and are referred to in the text. The “big picture is missing”

1 – Plots are described, not much else

0 – Major flaws, figures not described, etc.

**Conclusion:**

3 – The conclusion provides the final take away. Here is the big picture, why you wanted to read this paper. This plus the abstract would be enough to know why this is an important paper

2 – The conclusion provides the final take away. Does more than just summarize the results, but is still missing some of the importance and take away.

1 – Summarizes what was found.

0 – Where is the conclusion?

**Bibliography:**

2 – Everything is correctly cited

1 – Citations look weird or are missing

0 – Why are there no citations

You should probably use a citation manager for the references:

<https://www.zotero.org/>

<https://www.mendeley.com/>

The learning curve is not terrible, but it is much easier than managing the citations manually.

Some help on Gaussian

<http://gaussian.com/videos/>