Hydrogenative Depolymerization of Nylons

This paper (*J. Am. Chem. Soc.* **2020**, *142*, 14267) describes the activity of ruthenium catalysts with pincer ligands.

1) Carefully read the introduction and in your own words briefly (1 short paragraph) describe the significance of this study.

2) In the second paragraph of the introduction the authors say that the hydrogenation catalysis they are studying is "atom-economical, green, and sustainable". For now, focus on that first term, atom-economical. What do you think that term means? There are some additional hints to it in the rest of that sentence.

3) In the second paragraph, the authors begin to suggest a different name for nylons which includes a functional group that is important in their formation and this study. What is the term that is used and what is the important functional group?

4) Define polymers, oligomers and monomers. If you use an external source, be sure to cite it appropriately.

5) The authors state that they wish to do catalytic hydrogenation. Describe (meaning do not just copy) the particular reaction the authors wish to study in this paper. You might turn to Figure 1 for insight. Be sure to account for where the hydrogen goes in this catalytic hydrogenation.

6) Figure 1 B presents the different catalysts that were examined in this study. Using the CBC method, classify the catalysts, provide an electron count, the ligand bond number, the valence on ruthenium and the d^n count for ruthenium. Comment on any concerns you might have on the parameters. Upon classification, one of these catalysts is not like the others. Which one appears to be different, and how could you think about it in a way that would actually make it the same as the others?

7) The authors describe the catalysts as being ruthenium pincer complexes. What is a pincer and what makes it different from generic polydentate ligands?

8) The authors initially study the effect of different solvents on the catalysis. What were some of the difficulties the authors encountered with solvents and what was deemed good about the solvent they ultimately settled on.

9) After examining different solvents, the authors examined the activity of different catalysts. What particular reaction did they choose to study and what products did they observe?

10) Suggest a relative ranking of the different catalysts in terms of efficiency and provide support for your rankings. Some of this support should be inferred from

the data presented in Table 1 and some should be from the reasoning provided by the authors.

11) Once conditions were optimized, several different substrates were examined. Suggest a reason for the difference in activity for entries 1 and 2 in Table 2.

12) Compare entries 1 and 3 in Table 2. What conclusion could you possibly draw and what inherent risk is there in drawing this conclusion?

13) In Table 2, why are there two products listed under the selectivity heading for entries 4-8? Specifically, think about what the product(s) would be in entry 4.

14) What is the significance of entry 9?

15) The authors then examine the mechanism of the activity of this catalyst. What is the significance of studying the catalyst in the presence of KO^tBu, H_2 and DMSO?

16) Scheme 2 presents a proposed mechanism based on experimental and computational results. Parts of the experimental support are outlined in Scheme 1. Note that for clarity purposes, Scheme 2 does not show the CO ligand, but it is evident if you look at the calculated structures on the right side of this scheme. Describe what is happening in the steps going from compound **1** to D to C in Scheme 2. You might want to consider paying attention to the electron count and valence of the metal during these steps. Compound D is very similar to compound A in Scheme 1, just having undergone a shift of a hydrogen atom.

17) Scheme 2 shows the different considered transition state on the right side. For TS1, explain what the difference is between the two structures and which is the more likely for H_2 activation?

18) An interesting part of this study can be seen at the bottom of scheme 2. What does this suggest about the role of the metal in what the “important” reaction in this study.

19) The authors stated their desire to have a green, atom-economical process. Does this reaction entirely fulfill that goal?