

Paper 2 directions - possible useful information - CH 361 & CH 361H

3-4 pages is an ideal length (not counting Supporting Information or reaction diagrams). Supporting Information is not limited, but you should try to fit it into no more than 4 pages total.

The paper needs to be organized as a "Communication": the Experimental description and any calculations must go in an Appendix labeled "Supporting Information." If you fail to do this, you will be marked down for incorrect organization. Communications are short papers with a narrow focus on one or two things—like the synthetic reactions leading to your isomeric alkenes. This report goes through the simple distillation of the alkenes and does not include fractional distillation. It allows you to compare two synthetic strategies.

Abstract: Include reactions employed, grams of each of the alkene products, molar yield of each of the two alkenes produced, purity of isolated product (% 1-ene, % 2-ene), boiling range of each collected (crude) alkene mixture.

Introduction: Short overview of the two syntheses used to produce the alkenes. Include purpose for making the alkenes. You can include some brief discussion of both comparing the Grignard and Wittig reactions or other approaches, and use of traditional vs. ionic liquids as solvents (and the role they might play in the reaction). Both topics may also be handled in the later portion (Discussion) of the paper.

It is sensible to split the Results & Discussion section into two pieces: one dealing with each reaction. Be sure to show reactions (use ChemDraw or other software!) any time you talk about a reaction.

Grignard Section:

Give brief but detailed description of reaction including glassware used and conditions:

A. Grignard rxn to give alkoxide salt which was hydrolyzed to the alcohol Describe the experiment including compound additions & conditions & limiting reagents. Be sure to discuss undesired reactions and how the experimental design avoided (or minimized) these.

B. Separatory funnel workup NaHCO_3 & $\text{Na}_2\text{S}_2\text{O}_3$ Show the reactions that these reagents accomplish and explain why they had to be employed.

C. Distillation to remove ether - describe

D. Elimination reaction: Describe chemistry, catalyst used & type of distillation including conditions - head temp vs. distillate collected.

You want to explain how you calculated molar yield: $\text{mass-\% alkene in collected product mixture} \times \text{total mass collected} (= \text{g alkene}) / \text{MW alkene} = \text{moles alkene producte};$

$\text{molar yield} = \text{moles alkene produced} / \text{moles limiting reagent used}.$

Report yields of both 1-ene and 2-ene based on isolated mass and GC.

Wittig Section:

Give brief but detailed description of reaction including glassware used and conditions:

A. Describe assembly of the reaction setup and include masses/volumes and molar quantities of the reagents used. (BmimBF_4 is a solvent, not a reagent, but include the volume used only.)

B. Describe observations during the reaction period.

C. Describe the distillation—particularly the amount of heating used, and the relation between volume collected and head temperature.

D. Since GC's report mass percentages, calculate the following:

$$\text{Molar yield} = \frac{\text{mass of recovered mixture} \times \% \text{ alkene (from GC)}}{\text{MW alkene} \times \text{mol ketone used}} \times 100\%$$

$$\text{Conversion} = \frac{\% \text{ alkene in mixture}}{(\% \text{ alkene} + \% \text{ ketone})} \times 100\% \text{ (probably a bigger number)}$$

E. Be sure to reproduce the table of percentages from the GC report and identify each peak.

Experimental/Results: A formal Experimental section should be added **at the end as Supporting Information** (it can be called an Appendix). Please use a limited description in the body of the paper (to keep to the Communication format) but be sure to include all important details. Typically, a synthetic Experimental section can be condensed to one paragraph per compound.