

NOTEBOOK FORMAT  
CHEM 113A

Be sure to consult any handouts on the experiment before you begin the report.

I. Preparative Experiment

A. Heading. Give the experiment letter, title, your name and the date experimental work began.

B. Introduction. Prepare a brief, clear statement of your experimental objectives (2-3 sentences is usually sufficient).

C. References. List references to relevant background, procedures, physical constants, experimental variations, etc.

D. Main Reactions and Mechanism. Write the balanced equation for each reaction. Solvents, catalysts, reaction conditions, etc., should appear above or below the reaction arrow. Whenever possible, include the mechanism(s) below the balanced equation(s). Refer to your organic lecture text as necessary.

E. Side Reactions. If you are aware of any potential problems which will reduce the product yield and/or purity, a short discussion (or even better, balanced equation(s) and mechanism(s)) is appropriate. While not required for the preliminary report, some advance thought about side reactions may help you to improve on the experimental procedure. In the research laboratory such considerations are always evaluated in advance of performing an experiment.

F. Table of Starting Material and Products. List, in tabular form, each starting material under the following column headings: (see the sample report you were given for Experiment A as an example)

- (1) Compound
- (2) Molecular Weight
- (3) Amounts Used (subheadings for Weight, Volume and Moles)
- (4) Ratio of Moles (subheadings for Actual and Theoretical)
- (5) Physical Properties (include mp, bp, density, etc. as appropriate).

Note that the data in the text is generally not sufficient. There are two reference works with physical properties in the laboratory (the CRC Handbook of Chemistry and Physics and the Merck Index); you should learn how to use these. There are also on-line resources referenced on the course web site, such as the Aldrich Catalog.

Column (3) and the Actual Ratio of Moles obviously apply to starting materials only. The Theoretical Ratio of Moles is taken from the stoichiometric coefficients of the balanced equation for the main reaction. You should determine which is the "limiting reagent" by comparison of the Actual and Theoretical Ratios of Moles. It is the limiting reagent which determines the maximum amount of product which can be formed.

In all calculations, please pay attention to significant figures. However, the accuracy of your calculated values should never be limited by using values for constants (such as mol wt or density) which are not at least one digit more accurate than the least accurate of your "measured" values.

The table should also include catalysts, solvents, etc. , if their physical constants will be a matter of concern during the reaction or "work-up" (i.e., isolation and purification). For example, the boiling point of a solvent will be useful if the product is later to be separated from it by distillation.

G. Limiting Reagent. State which starting material, if any, is the limiting reagent.

H. Yield Data. Show your calculations for theoretical yield. Leave a space to insert the percentage yield when your actual yield has been determined. (See Lehman, Appendix IV)

I. Method of Purification. A very important phase of synthetic organic chemistry is the separation and purification of the desired product. Because of the many and varied reactions that organic compounds undergo, frequently the most difficult step in the preparation of a compound is not its actual formation but its isolation in pure form from byproducts, side products and unchanged starting materials. To accomplish this, determine all the compounds that could possibly be present on the basis of a consideration of the main and side reactions. Devise a purification scheme, using a flow chart to see how various purification procedures eliminate the undesired substances and yield the pure product. By examining a purification scheme in this manner, the purpose of each step in the procedure becomes clear, and one may be able to predict what impurities, if any, may contaminate the product.

Many hyper-linked flow diagrams are provided on the web site. If available, this may be copied into the notebook.

**YOUR NOTEBOOK MUST BE COMPLETED UP TO THIS POINT (except section E which may be completed later) AND SUBMITTED FOR APPROVAL PRIOR TO GETTING YOUR STARTING MATERIAL FOR THE EXPERIMENT. YOU MUST ALSO HAVE THE RELEVANT PORTIONS OF THE LAB REPORT SUMMARY (COVER SHEET) FILLED OUT TO BE SIGNED BY THE INSTRUCTOR BEFORE YOU MAY PROCEED.**

J. Observations, Data and Notes. During the experiment all such information should be recorded directly in the notebook (not transferred from other notebooks or scraps of paper, or recreated from memory at a later date). Record all significant observations that you make, but be sure to point out any deviations from or difficulties with a published experimental procedure. Observed physical properties of your product(s) should always be accurately reported. Always record mp and bp as ranges (e.g., mp 123-4°C). Much of chromatographic and spectral information is shown directly on the charts. However, this section of your notebook is the appropriate place to tabulate and assign these data. Calculations should be shown at the end of this section and not in the conclusions section.

All notebook entries should be dated.

K. Conclusions. Unlike the above sections, which are entered by hand in the lab notebook, the conclusions will be submitted as a text file to a web site (turnitin.com - details to be provided) and a double-spaced printed copy will be attached to the report. (The printed copy and the on-line submission must be identical.) After completing the assigned experiments, state concisely and in your own words the conclusions which you have reached on the basis of the results you obtained. You may wish to discuss possible reasons for product loss or to suggest improvements in the procedure. If the experiment was the identification of an unknown, summarize the results of the findings here along with a concise account of the logic used to arrive at your conclusion.

It is crucial to observe the distinction between observations and conclusions. Observations (see above) are made in the lab. Conclusions may be made leisurely and thoughtfully in the comfort of a non-lab environment.

Unless otherwise stated, the conclusions section should never exceed four double-spaced pages. Often less is sufficient. It is advisable that you form an outline of your conclusions before you begin writing them.

Although you will restate and discuss key data in the conclusions section (in some cases a table of key results may be appropriate) this is not the place for calculations. Calculations are best done at the end of the Observations section (Sec. J). Yield calculations may be done at the bottom of the Table of Starting Materials and Products (Sec. F).

(...see next page for Investigative experiment format...)

II. Investigative Experiment. The experimental write-up is essentially the same as for a preparative experiment, except that sections D, E, F, G and H may be omitted as appropriate; this is for you to judge. You must have a table of physical properties (Section F) of any reagents/solvents that you use (Section I, method of purification, will be necessary in many cases). Typically, sections B (Introduction), J (Observations) and K (Conclusions) will be a bit more lengthy than for a preparative report; the exact nature of the experiment will dictate the relative emphasis each section deserves in the write-up.

### III. Some General Notes.

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Experiments involving unknowns: Either preparative or investigative experiments may involve unknowns. Be sure to record the unknown number directly in the lab notebook when it is issued. Write it also on the Lab Report Summary sheet and at the beginning of your conclusions section.

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Submitting lab reports: Lab reports are to be handed in by the **beginning** of the lab period on which they are due (see Greensheet). Staple them in the following order: Lab Report Summary sheet, notebook page carbons, any spectra or other material. Be sure your name is on the Lab Report Summary sheet and on the first page of your report.