

Massachusetts Institute of Technology
Organic Chemistry 5.13

Wednesday, February 27, 2002

Prof. Timothy F. Jamison

Hour Exam #1

Name Solutions
(please both print and sign your name)

Recitation Instructor _____

Directions: Closed book exam, no books, notebooks, notes, etc. allowed.
However, calculators and molecular model sets **are** permitted.

Please read through the entire exam before beginning, in order to make sure that you have all the pages and in order to gauge the relative difficulty of each question. Budget your time accordingly.

Show all of your work if you wish to receive partial credit.

You should have 11 pages total: 5 exam pages including this page, 4 pages of reference information, and 2 blank pages for scratchwork.

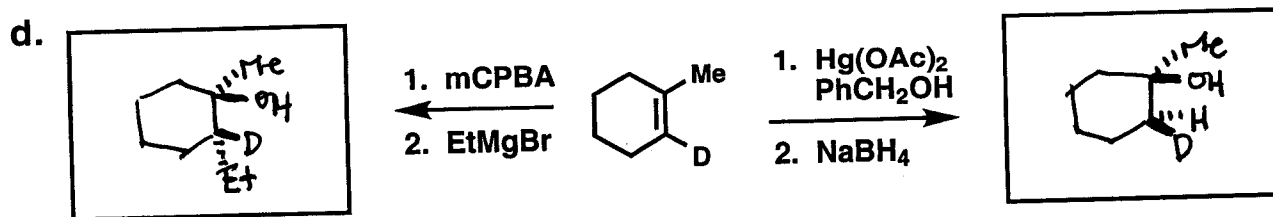
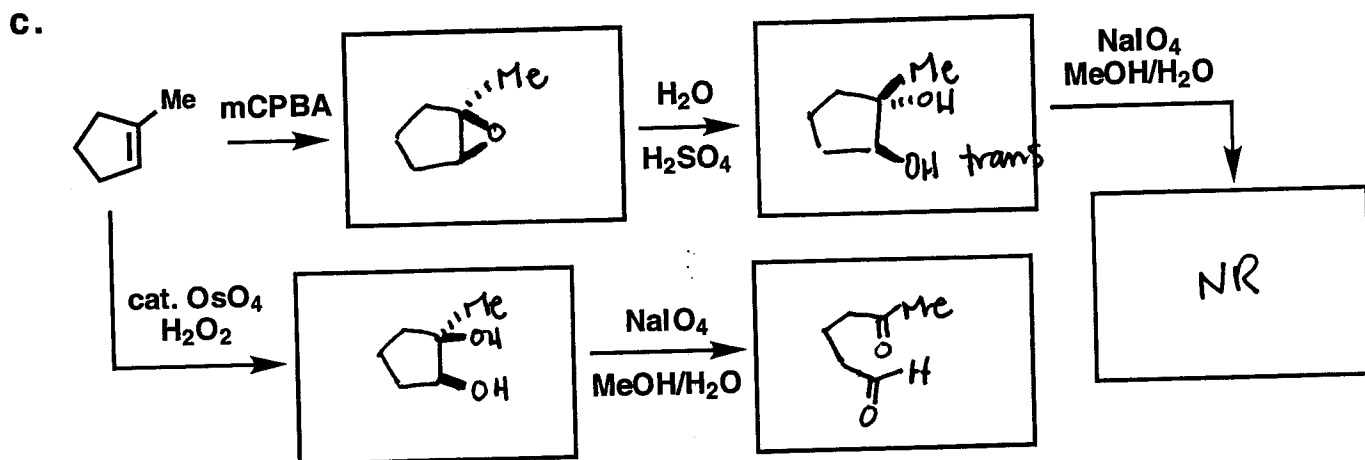
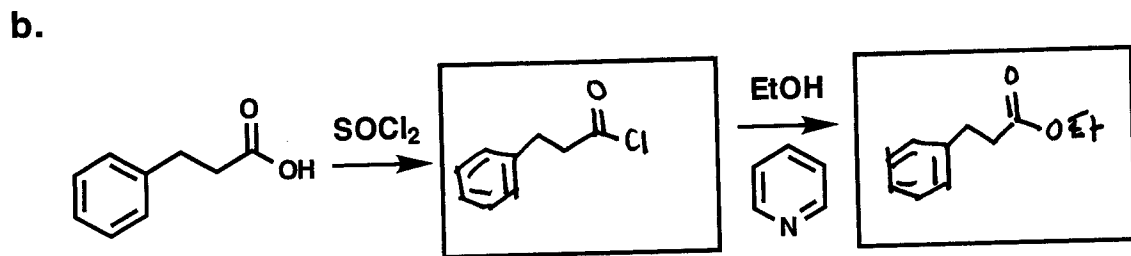
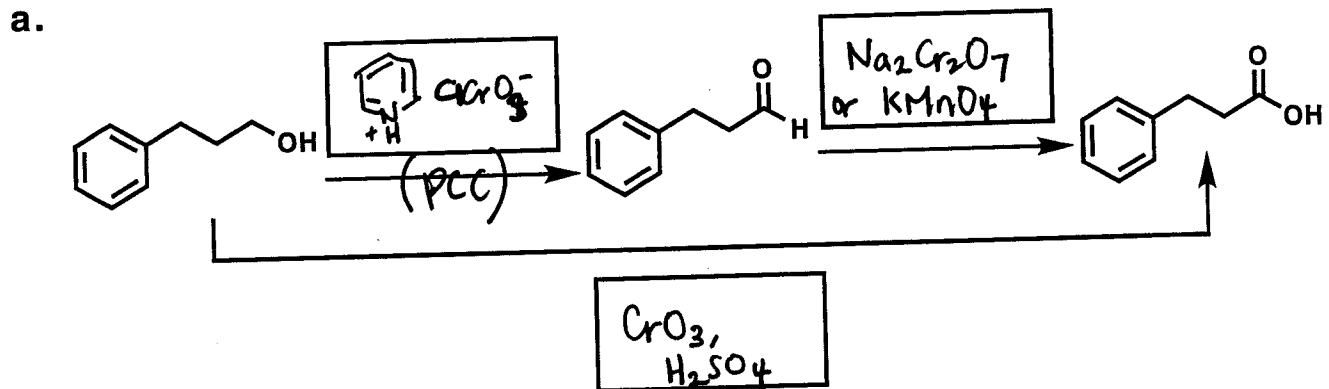
Question:

Grader:

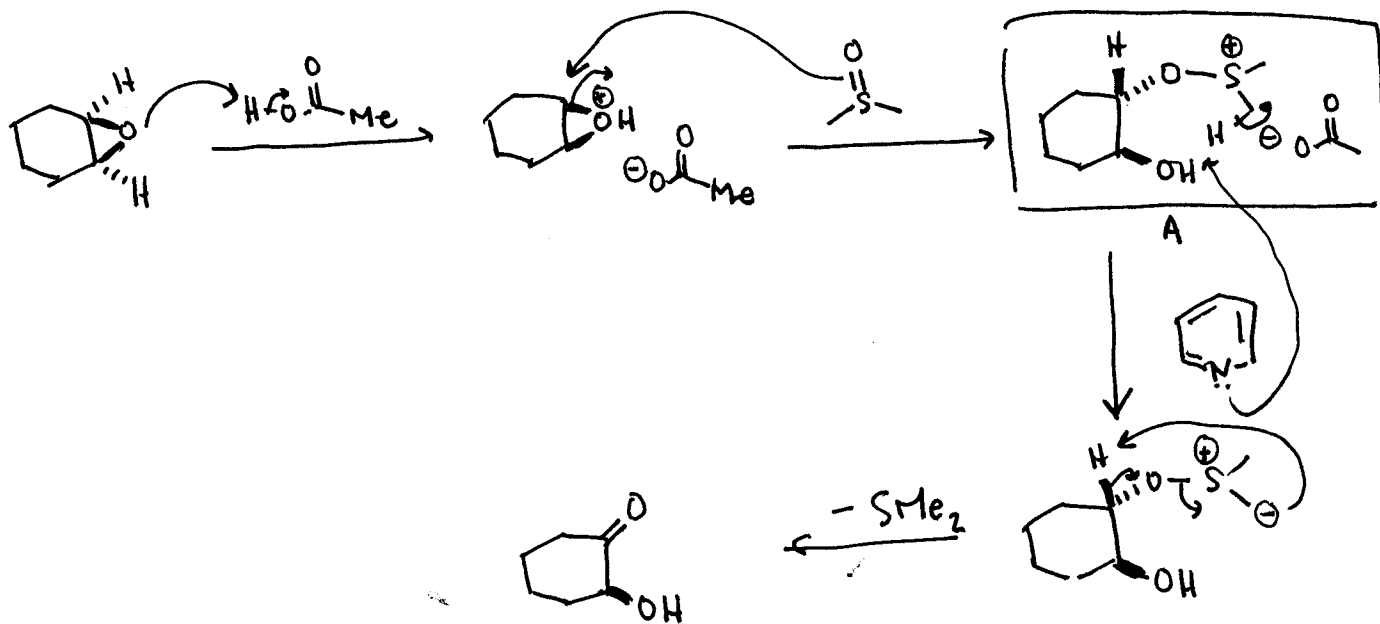
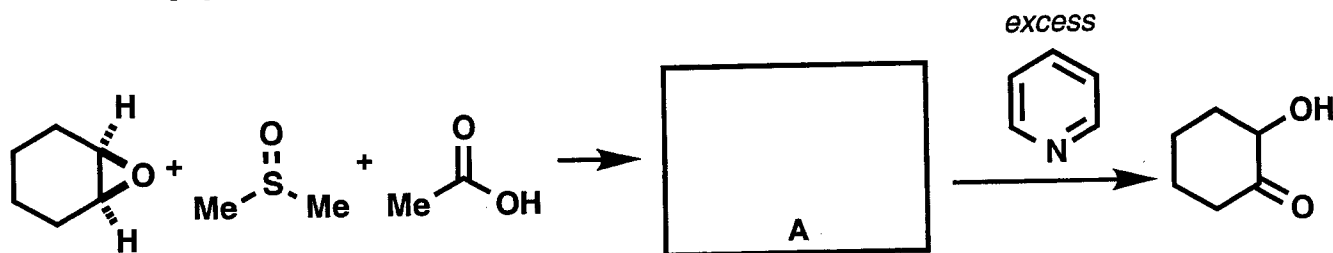
1. _____/	12 points	_____
2. _____/	20 points	_____
3. _____/	36 points	_____
4. _____/	32 points	_____

Total: _____/ 100 points

1. (12 points, 1 point per box) In the boxes below, write the product of the reaction indicated or the reagent or reagents (e.g. not "Jones Reagent") required for the transformations shown. Where relevant, clearly indicate stereochemistry. If no reaction occurs, write "no reaction" in the box.



2. (20 points) In the reaction shown below, an epoxide is converted to a hydroxyketone in two steps. Write the structure of the epoxide-derived product of the first reaction (compound **A**) in the box below. In the space below the reaction, **clearly** write an arrow-pushing mechanism for **both steps** (i.e. starting materials \rightarrow compound **A** \rightarrow products). Clearly draw all **intermediates** and **reaction by-products** in your mechanism.



3. (36 points, 6 points each) As part of a Ph.D. thesis, an MIT graduate student performed a reaction in the lab in which a foul-smelling organic molecule (compound **A**) was treated with **NaOH** and **CH₃I**, giving compound **B**, which had a slightly less offensive odor. Some of the spectral data for compound **B** are listed below. If applicable, **clearly** indicate the **geometry of all alkenes** (e.g. cis or trans). (MW of S = 32.06)

EA: C, 67.69%; H, 6.49%; S, 25.82%

MS: M⁺ = 124

¹H NMR (ppm) 7.18 (2H, dd, J = 2, 8), 7.16 (2H, dd, J = 7, 8), 7.02 (1H, dd, J = 2, 7), 2.47 (3H, s)

a. What is the molecular formula of compound **B**?



b. What is the "index of hydrogen deficiency" of compound **B**? (Hint: Treat sulfur as you would oxygen in such a calculation)

$$IHD = 4$$

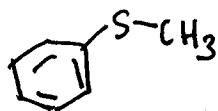
c. How many chemically nonequivalent **carbon** atoms does compound **B** have?

5

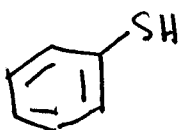
d. How many chemically nonequivalent **hydrogen** atoms does compound **B** have?

4

e. Draw the structure of compound **B**.



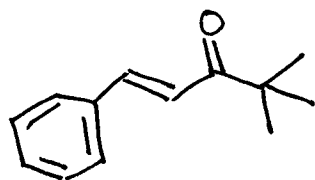
f. Draw the structure of compound **A** (the foul-smelling starting material).



4. (32 points) In the box below, draw the structure of the unknown compound having MF $C_{13}H_{16}O$ and the 1H NMR data below. If applicable, clearly indicate the geometry of all alkenes (e.g. cis or trans).

1H NMR (ppm) 7.54 (1H, d, $J = 16$), 7.30 (2H, dd, $J = 2, 8$), 7.21 (2H, dd, $J = 7, 8$), 7.14 (1H, dd, $J = 2, 7$), 6.67 (1H, d, $J = 16$), 1.21 (9H, s)

Your proposed structure:



trans double bond.