

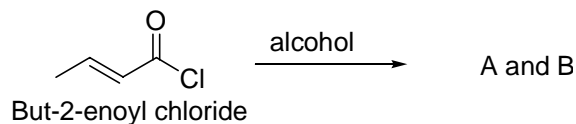
PreLab assignments are due at 1 pm before lecture – Feb 17 TR section; Feb 18 WF section. This pre-lab contains only three questions. You should be able to answer each question with the aid of your lab manual, Chapter 19 in Mohrig text, and your organic text. There are 2 pages. NMR is the topic for the lecture this week.

1. (2 pts) Calculate a value for the ΔH_f^0 for ethylene oxide (C_2H_4O) given that the measured ΔH_c^0 from calorimetry is -1310 kJ/mol (hint: see eq 8 for Expt 2 in the lab manual). How does this experimental value for ΔH_f^0 compare to a value of -37.7 kJ/mol for a calculated ΔH_f^0 using HyperChem? (Give a % comparison based on the measured value as the true value.) The HyperChem value was determined for the best geometrically optimized structure of ethylene oxide using the PM3 semi-empirical method. (Hint: you have to balance the combustion reaction.)

2. (2 pts) Write the structural formulae for the tautomers for (a) acetone and (b) phenol.

3. (2 pts) In order to make a 0.5mL solution of a 0.10 mole fraction solution of 2,4-pentanedione (Hacac) in d-6 DMSO ($(CD_3)_2SO$), what volumes of Hacac and $(CD_3)_2SO$ are needed to prepare the solution? Please show your calculations and results for the volume of both components below. Note: Hacac: MW = 100.11 g/mol; density = 0.98 g/mL; $(CD_3)_2SO$: MW = 84.18 g/mol; density = 1.19 g/mL

4. (3 pts)



A student takes but-2-enoyl chloride and reacts it with what was thought to be a pure alcohol (C_3H_8O), but in fact it was a mixture of two alcohols (C_3H_8O), and finds two products (A and B). These compounds were isolated and 1H NMR was run on both samples for structure determination (see data below).

Draw two structures that conform to known chemistry for A and B that are supported by this NMR data and label the protons on each structure to show which signal they produce in the 1H NMR.

| Compound A | | | |
|-------------------|---------------------------|-------------|----------------|
| Peak | Splitting pattern / Peaks | Integration | Chemical shift |
| 1 | Doublet / 2 | 3H | 1.9 |
| 2 | Multiplet* / 8 | 1H | 6.2 |
| 3 | Doublet / 2 | 1H | 5.8 |
| 4 | Septet / 7 | 1H | 5.1 |
| 5 | Doublet / 2 | 6H | 1.2 |

*doublet of quartet

| Compound B | | | |
|-------------------|---------------------------|-------------|----------------|
| Peak | Splitting pattern / Peaks | Integration | Chemical shift |
| 1 | Doublet / 2 | 3H | 1.9 |
| 2 | Multiplet* / 8 | 1H | 6.2 |
| 3 | Doublet / 2 | 1H | 5.8 |
| 4 | Triplet / 3 | 2H | 4.9 |
| 5 | Multiplet** / 12 | 2H | 1.8 |
| 6 | Triplet / 3 | 3H | 1.2 |

*doublet of quartet ; **triplet of quartet

Structure A:

Structure B:

5. (1 pts) Show on the diagram below which direction is called “upfield” and which is called “downfield” from a value of 6 ppm in this example.

