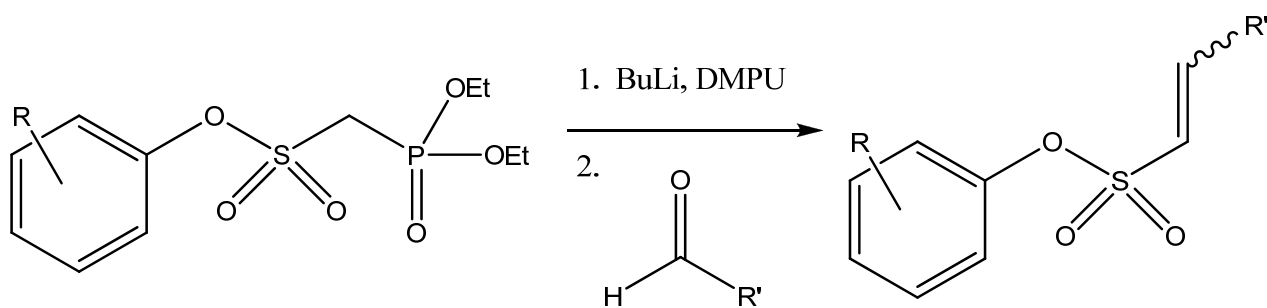


## Identification of an Unknown Sulfonate Ester

Purpose: Use spectra and data provided to determine the structure of an unknown sulfonate ester

Background: In this DRY LAB, we will be simulating this event:

Fred Chemist has tried to carry out one of the reactions in your proposal, and has successfully synthesized an aryl sulfonate ester. (Congratulations!) His joy is short-lived however, when he realizes he forgot to write in his lab notebook the identity of the sulfonate and aldehyde he used (Fig 1.)



He was able to obtain a decent yield of only one isomer, however. He obtained proton NMR,  $^{13}\text{C}$  NMR, and high resolution GC-MS. In a separate experiment, he determined the structure to be 56.58% carbon and 5.70% hydrogen by elemental analysis.

In this lab, you will inspect the data he collected and determine a structure that is consistent with the data. When you walk into lab, you will do check-out, then you will be given the data. Work by yourself or with one partner (no more!) to fill in the following sheets. Turn them in to your AI before leaving. There is no additional report or lab notebook to fill out!

Names of Partners \_\_\_\_\_

1. Molecular Formula: \_\_\_\_\_

2. Explain the way you determined the molecular formula, giving reference to the data. Is all the data consistent with your molecular formula?

3. Draw a proposed structure of compound, with all coupling constants from the  $^1\text{H}$  NMR :

4. How did you determine if the alkene was (E) or (Z)?

5. Is the carbon-13 NMR consistent with this structure? Explain any inconsistencies.
  
  
  
  
  
  
  
  
  
  
6. In what two ways do the data suggest that Fred's sample is not 100% pure?
  
  
  
  
  
  
  
  
  
  
7. Draw your structure on the full proton NMR. Label the protons in your structure A-E to correspond to the NMR. Attach the spectrum to this handin sheet.
  
  
  
  
  
  
  
  
  
  
8. Describe the signal at about 7.1 ppm and describe how the coupling fits your proposed structure.
  
  
  
  
  
  
  
  
  
  
9. Describe the signal at about 6.5 ppm and describe how the coupling fits your proposed structure.
  
  
  
  
  
  
  
  
  
  
10. Describe the signal at about 2.5 ppm and describe how the coupling fits your proposed structure.