

Massachusetts Institute of Technology

Organic Chemistry 5.13

September 15, 2006  
Prof. Timothy F. Jamison

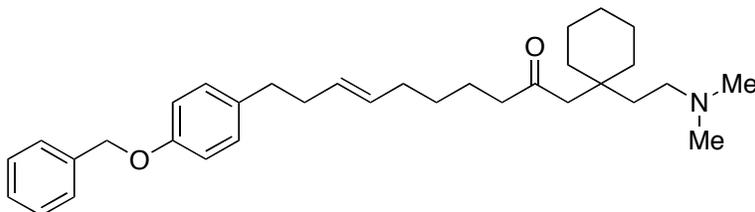
Problem Set #2

This problem set is worth 50/8 = **6.25 points** toward your final grade; each problem is worth **1.25 points**.

**DUE DATE: Friday, September 22, 2006, in lecture, before lecture (at 12:05 p.m.).**

NOTE: If mass spectrometry (MS) data are provided, the highest molecular ion given corresponds to the molecular ion ( $M^+$ ), unless otherwise noted.

1. Predict **10**  $m/z$  values that you would expect to see in an MS of the following compound. Using the convention presented in class, indicate the site (and value) of each fragmentation on your drawing of the structure.

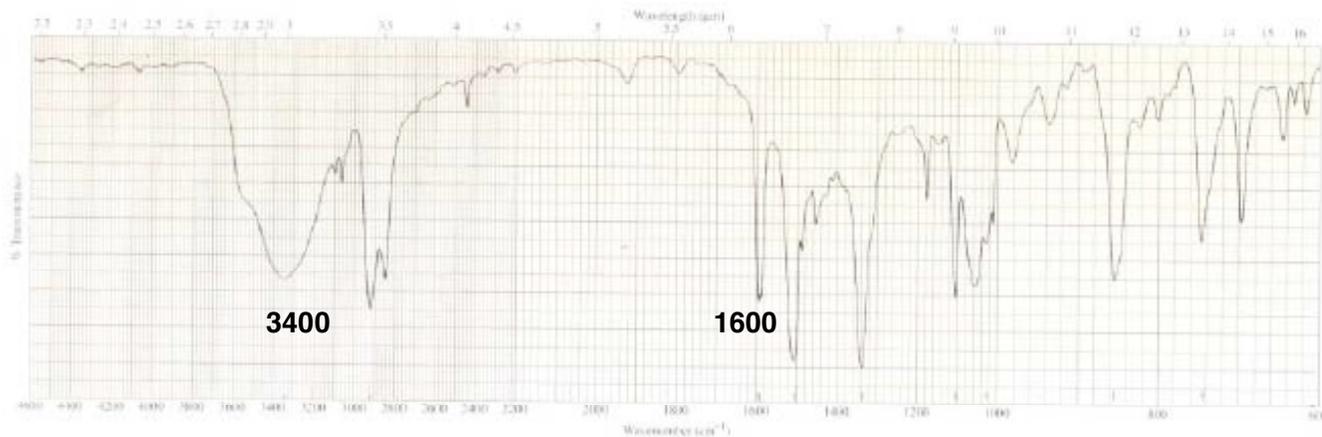


2. The **Wittig Reaction** (McMurry, pp 706-708) is one of the most reliable methods for the stereoselective preparation of alkenes.
  - a. Propose a synthesis of *cis*-3-octene using the Wittig reaction as the final step and no starting material with more than 5 carbon atoms, except for Ph<sub>3</sub>P.
  - b. What other product(s) may be formed in the Wittig reaction?
  - c. What spectroscopic method(s) would allow you to differentiate between/among these different products? List the methods and the key data values for your determination.
  - d. Propose a **chemical** means by which you could confirm your assignment in (c).

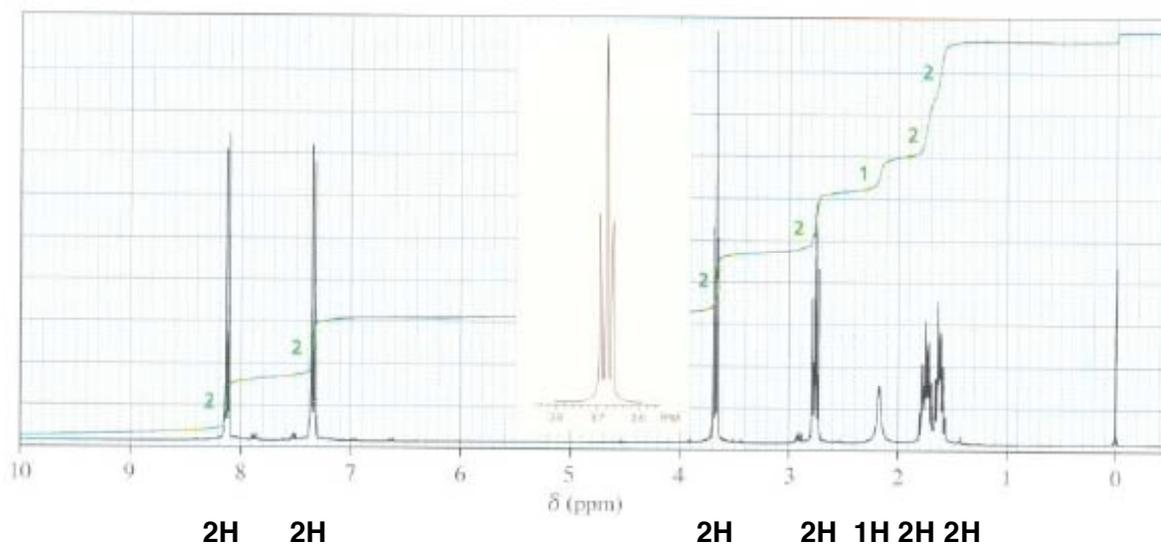
3. Draw the structure of the compound that satisfies the following experimental data and is consistent with the spectra provided below. (I apologize for the poor resolution of these spectra. I have highlighted some key areas and data in each spectrum.)

EA (found): C, 61.53; H, 6.71; N, 7.18.

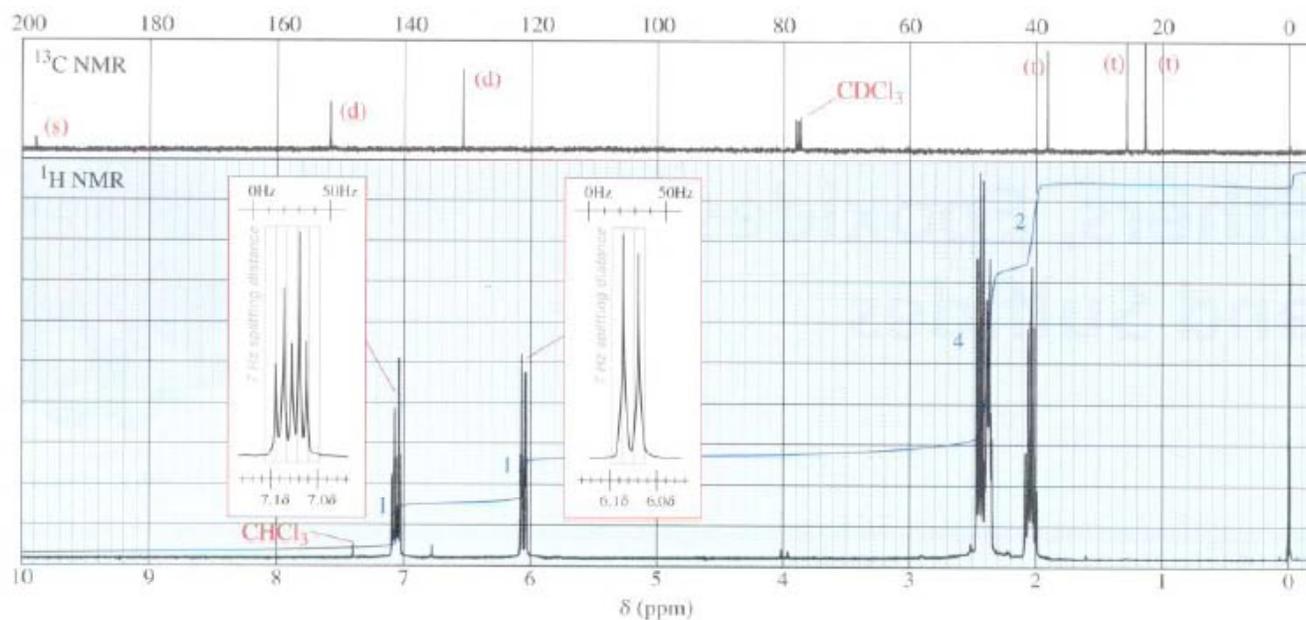
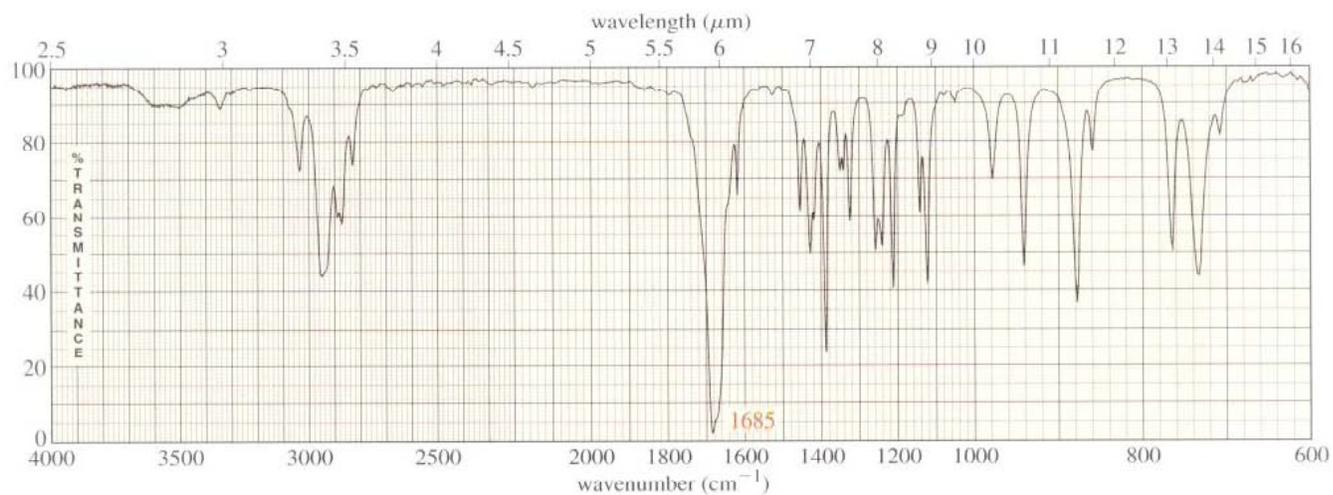
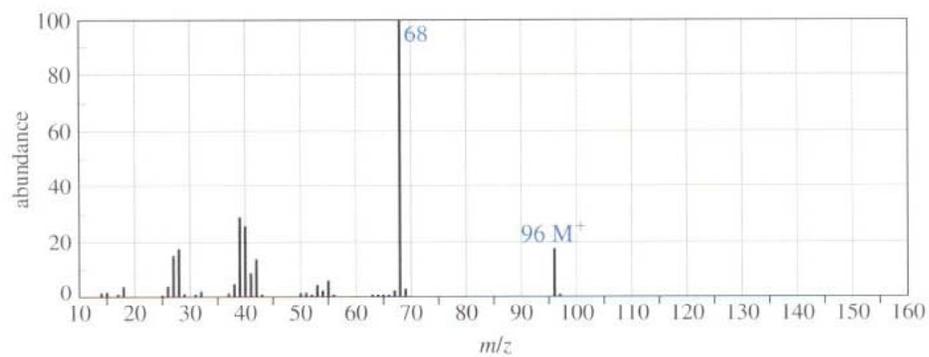
MS: 195



*expansion of 3.9 to 3.5 ppm*

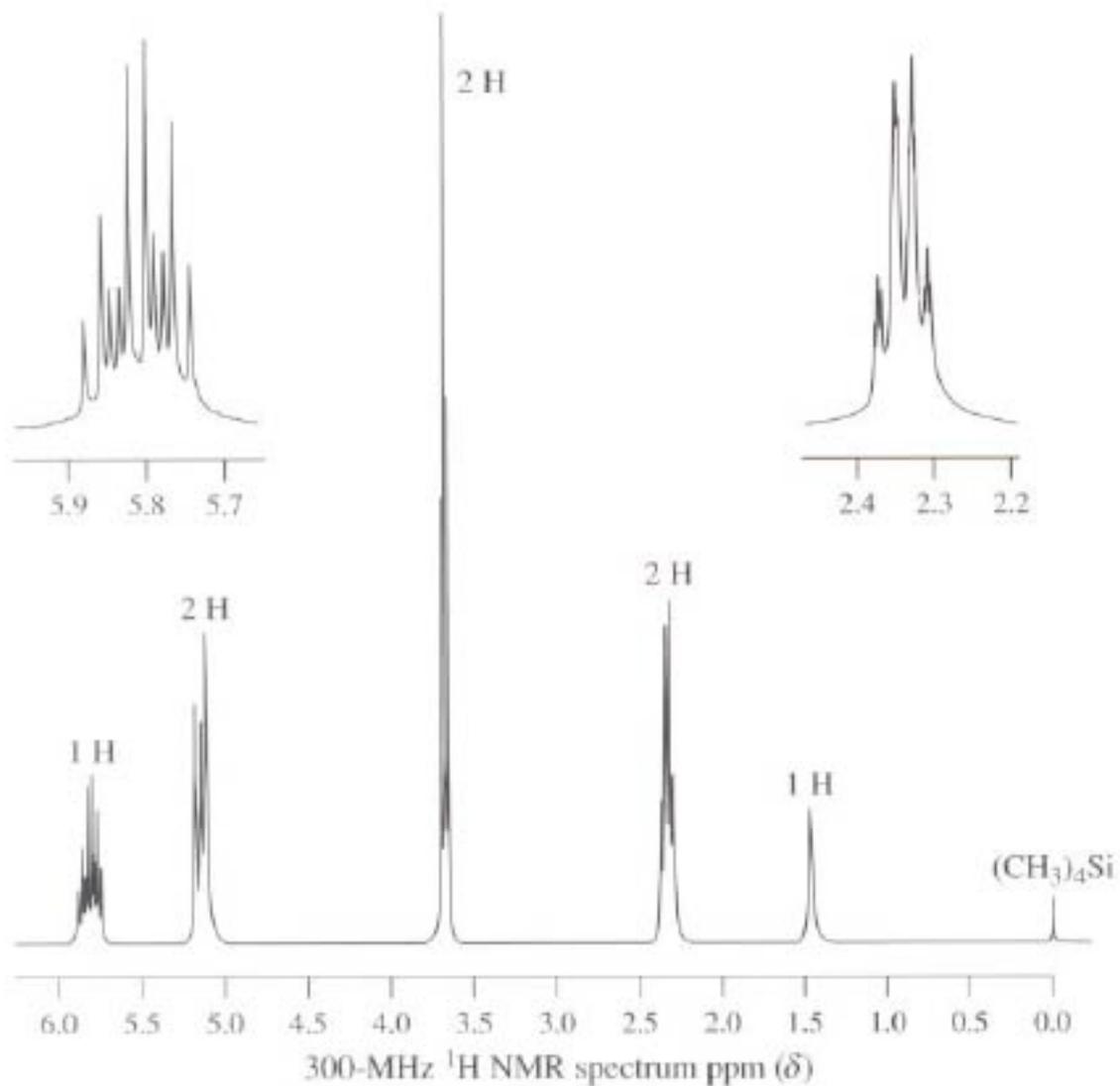


4. Draw the structure of the molecule consistent with the spectra provided below.



5. The  $^1\text{H}$  NMR spectra of two molecules with the **same** molecular formula and a MW of **72** are given below. Determine the structure of each compound.

a.



b.

