Massachusetts Institute of Technology
Organic Chemistry 5.13

Friday, September 29, 2006 Prof. Timothy F. Jamison

Hour Exam #1

Name ____

(please both **print** and **sign** your name)

<u>Official</u> Recitation Instructor ______________________________

Directions: *Closed book exam, no books, notebooks, notes, etc. allowed. However, calculators, rulers, 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 **14** pages total: **8** exam pages including this page, **4** pages of reference information, and **2** blank pages for scratchwork.

Question:		**Grader:**
1. ________/	**10 points**	_______
2. ________/	**25 points**	_______
3. ________/	**25 points**	_______
4. ________/	**25 points**	_______
5. ________/	**15 points**	_______
Total: ________/	**100 points**	_______

1. **(10 points total, 2 points each)** For each set of compounds below, **circle** the one in which the indicated hydrogen is the **furthest <u>upfield</u>** in a ^{1}H NMR spectrum.

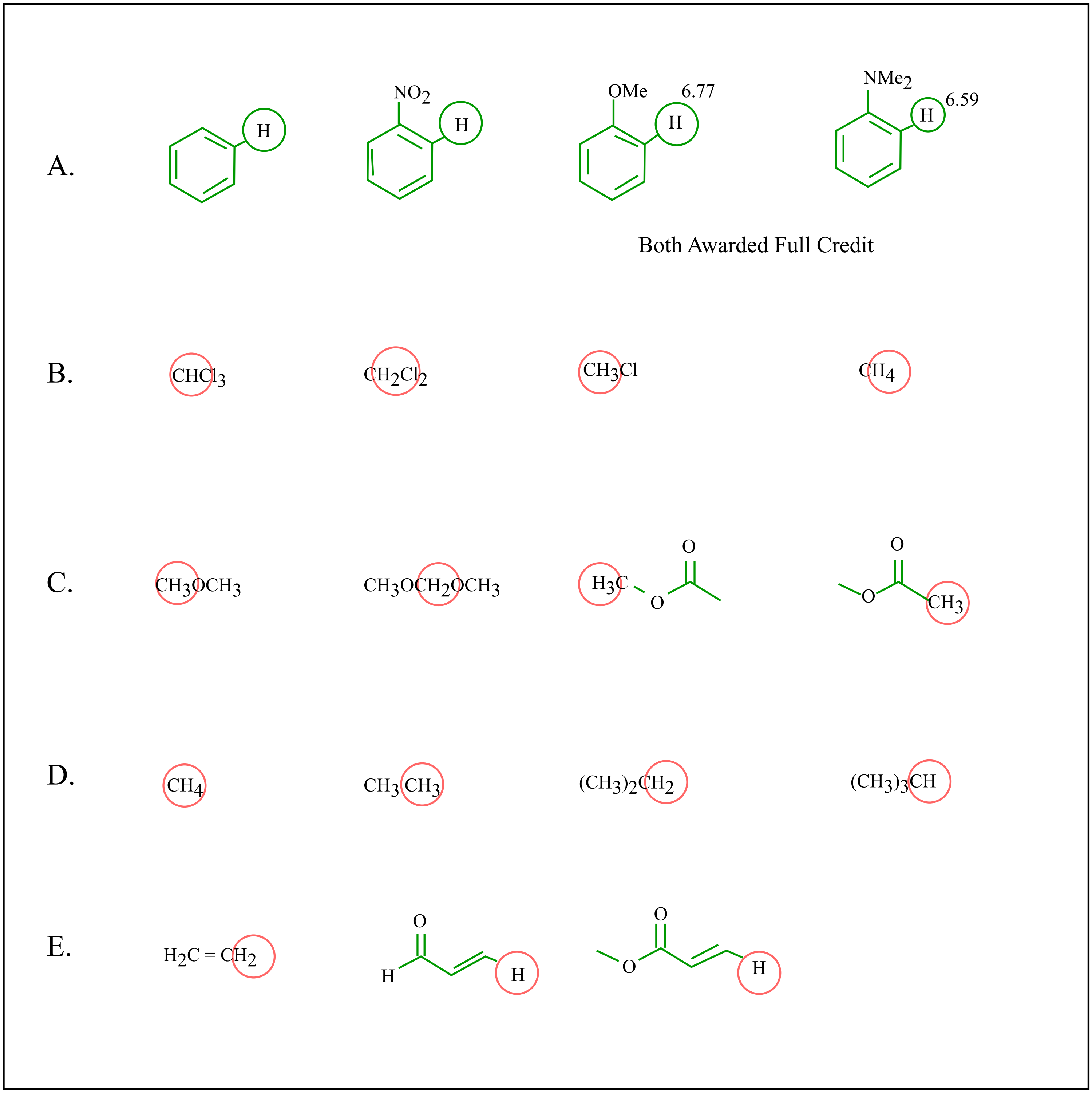


Figure by MIT OCW.

2. (25 points total) Answer the questions below about the structure that has the following data:

EA	C, 66.62; H, 11.18; N, 22.20
MW (g/mol)	126.20
^{13}C NMR (ppm)	140.3, 49.0, 24.7
IR (cm^{-1})	2116 (strong – more intense than the C–H stretches between 2800 and 3100); no other peaks between 1500 and 4000.

^{1}H NMR spectrum:

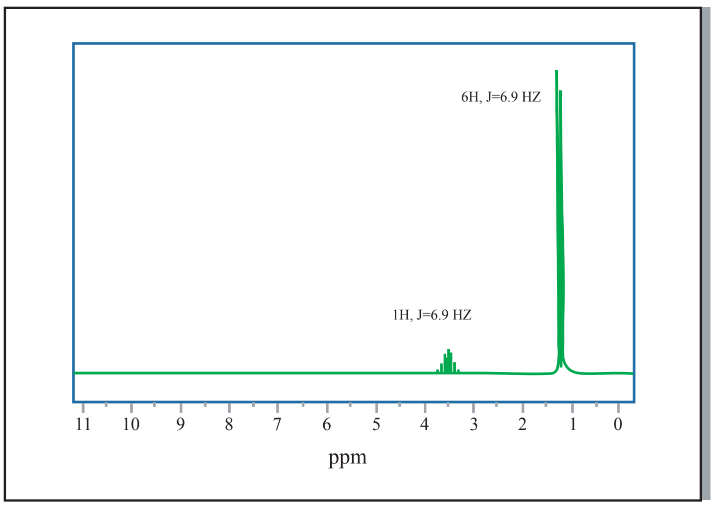


Figure by MIT OCW.

a. (3 points) To what structural fragment does the signature splitting pattern in the ^{1}H NMR correspond? **Circle** your final answer.

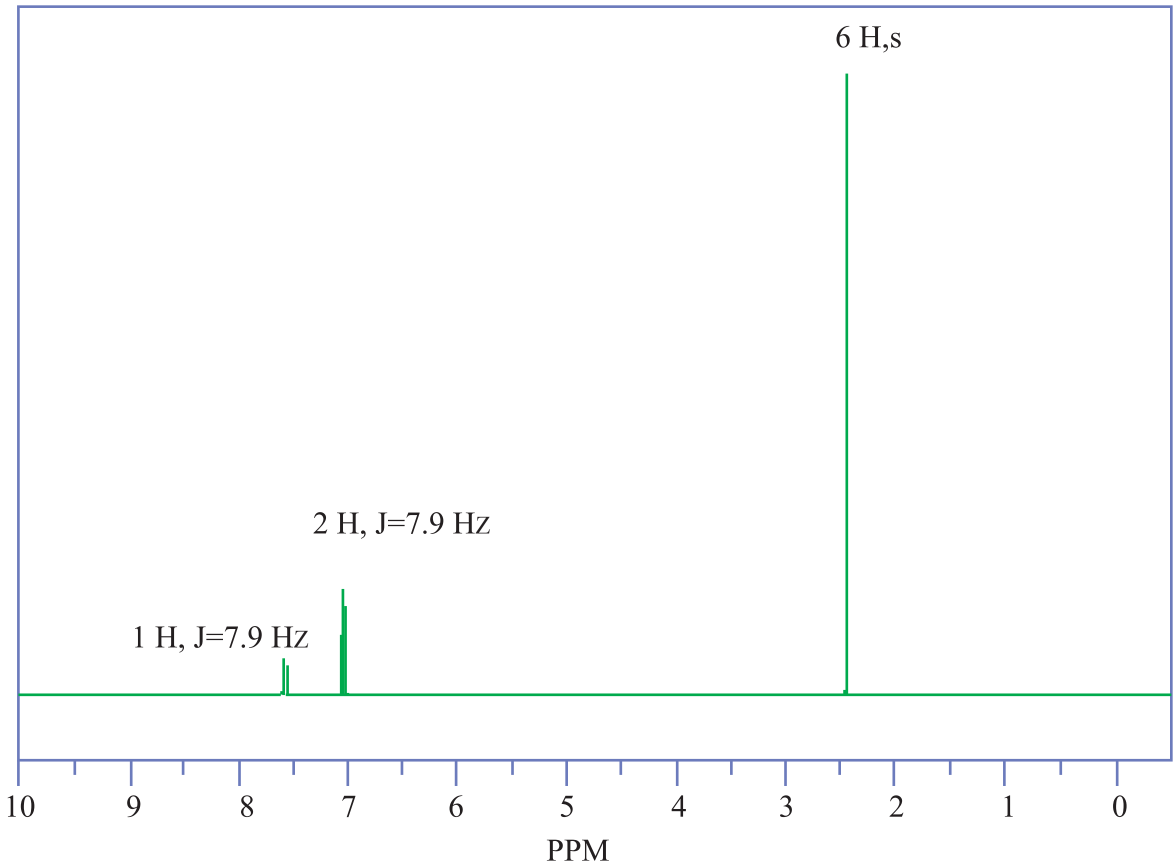
b. (2 points) Which peak or peaks in the ^{13}C NMR correspond(s) to the fragment you identified in **a**, above. List the chemical shift(s) of the peak(s), and **circle** your final answer(s).

c. (5 points) Determine the molecular formula of this compound. **Circle** your final answer.

d. (5 points) Calculate the Index of Hydrogen Deficiency (IHD) of this unknown compound. **Circle** your final answer.

e. (10 points) **Draw** the structure of the unknown compound. **Circle** your final answer.

3. (25 points total) Answer the questions below about the structure that has **MW = 107** and the following NMR spectra:



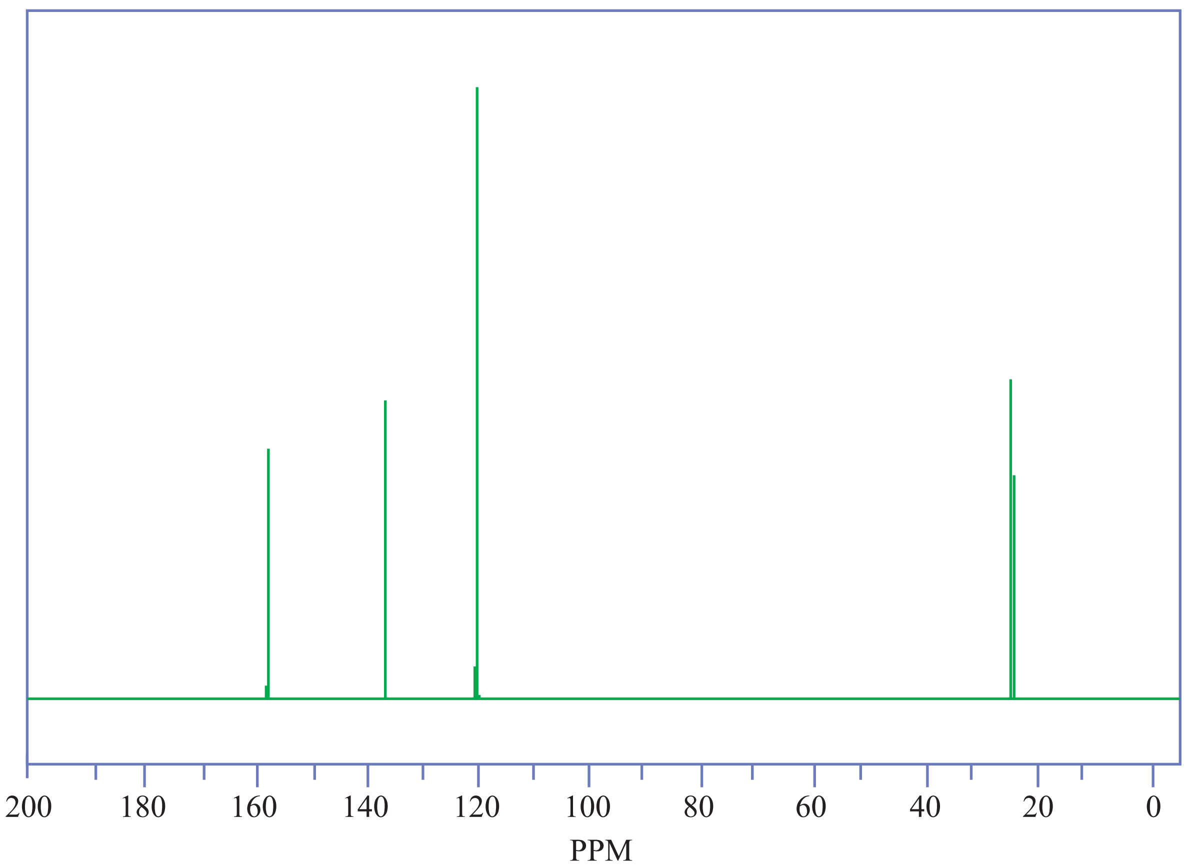


Figure by MIT OCW.

a. (10 points) Determine the molecular formula of this compound. **Circle** your final answer.

b. (5 points) Calculate the Index of Hydrogen Deficiency (IHD) of this compound. **Circle** your final answer.

c. (10 points) **Draw** the structure of the unknown compound. **Circle** your final answer.

4. (25 points total) An unknown compound (**X**) contains **only** carbon and hydrogen, has MW = 112, and exhibits the spectral data below. In addition to the IR signal listed below, there are only peaks corresponding to C–H stretches (between 3300 and 2900) and several peaks in the "fingerprint region". Please note that there are no overlapping peaks in either the ^{1}H NMR or the ^{13}C NMR spectra. In other words, "What you see is all there is!"

IR (cm^{-1})	2145
^{13}C NMR (ppm)	77.8, 70.1, 30.2
^{1}H NMR (ppm)	2.45 (s)

When compound **X** was treated with excess *n*-BuLi (*n*-butyllithium) in tetrahydrofuran and then excess CH_3I (iodomethane), a new compound (**Y**) with MW = 168 and 4 signals in its ^{13}C NMR spectrum was formed.

What are the structures of **X** (15 points) and **Y** (10 points)? (Show your work in the space below for partial credit consideration.) Write your final answers **in the boxes provided** below.

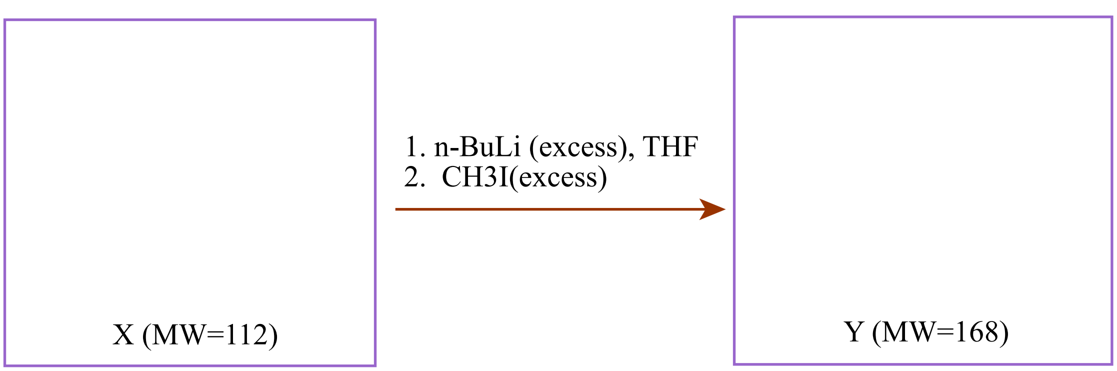
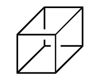


Figure by MIT OCW.

5. (15 points) In one of our problem sets, cubane (C_8H_8) was one of the possible answers to a structure elucidation problem. Based on the formula for the Index of Hydrogen Deficiency, the IHD of cubane is **5**. However, as you know, a cube has six sides. In other words, it looks like cubane has 6 rings and thus that its IHD should also be 6.



cubane

C_8H_8
IHD = 5

Please provide an explanation (**not** the formula used to calculate the IHD) for this apparent discrepancy in the space below.