ORGANIC CHEMISTRY 136

(Prof. Yves Rubin)

UCLA, SPRING 2011

FINAL EXAM

_____

Please print your name

Question	Points
1 (20)	
2 (20)	
3 (50)	
4 (40)	
5 (50)	
6 (20)	

Total **(/200)**

==========

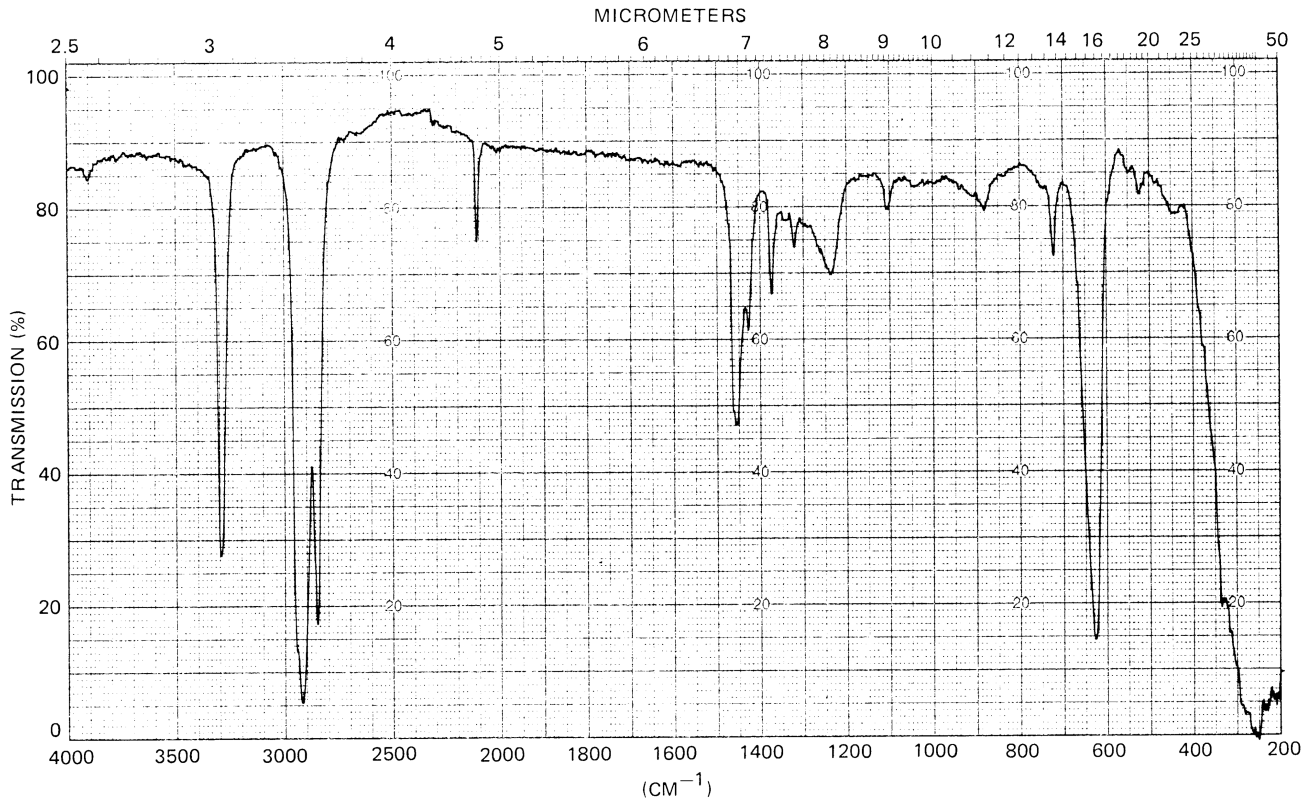
Name _____

1. (20 points) Assign all IR-absorption bands you can recognize as meaningful and informative for an unknown compound with molecular formula (C_8H_{14}) and provide its structure:

Compound C_8H_{14}

(use as many lines as necessary)

Infrared spectrum (neat)



Name _____

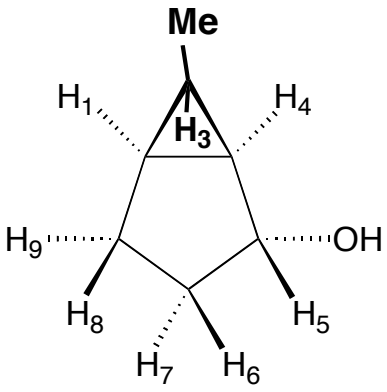
2. (20 points) Estimate the **dihedral angles** (e.g. 130°) and corresponding **coupling constants** for the following compound using the Karplus relationship shown below or other sources if necessary. Be sure to consider all factors affecting these parameters:

a) Dihedral angle (H_1-C-C-H_4): _____ $J_{1,4}$: _____

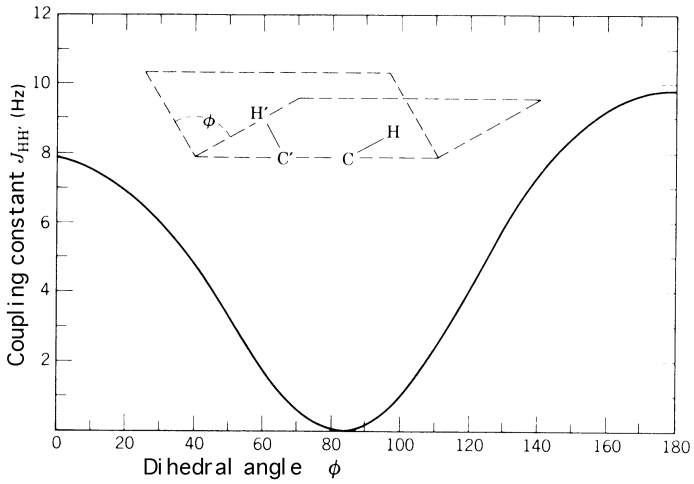
b) Dihedral angle (H_4-C-C-H_5): _____ $J_{4,5}$: _____

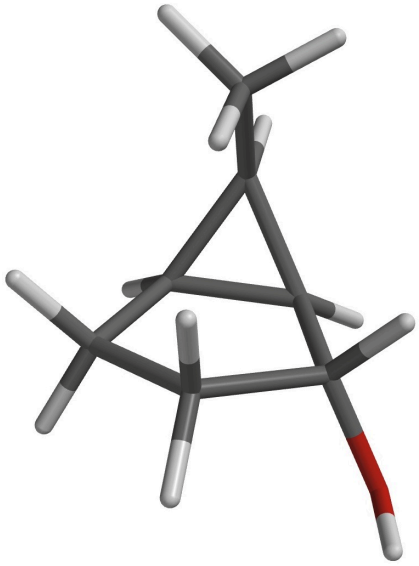
c) Dihedral angle (H_5-C-C-H_7): _____ $J_{5,7}$: _____

d) Dihedral angle (H_6-C-C-H_8): _____ $J_{6,8}$: _____



e) Other than for *geminal* and *vicinal* protons, draw a curved double-headed arrow for **the strongest** NOE enhancement you expect to observe with this molecule

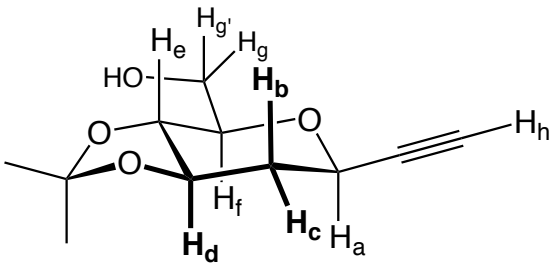




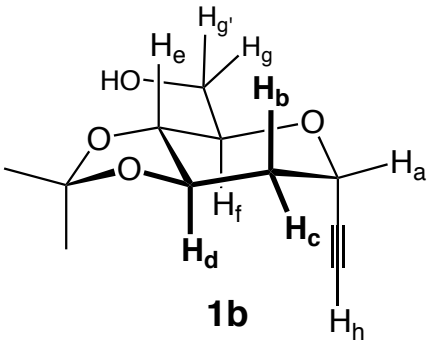
(calculated structure)

Name

3. (50 points). a) (20 points) Describe *two* distinct NMR techniques that will help differentiate and assign the diastereomers **1a** and **1b**:



1a



1b

Technique 1:

Technique 2:

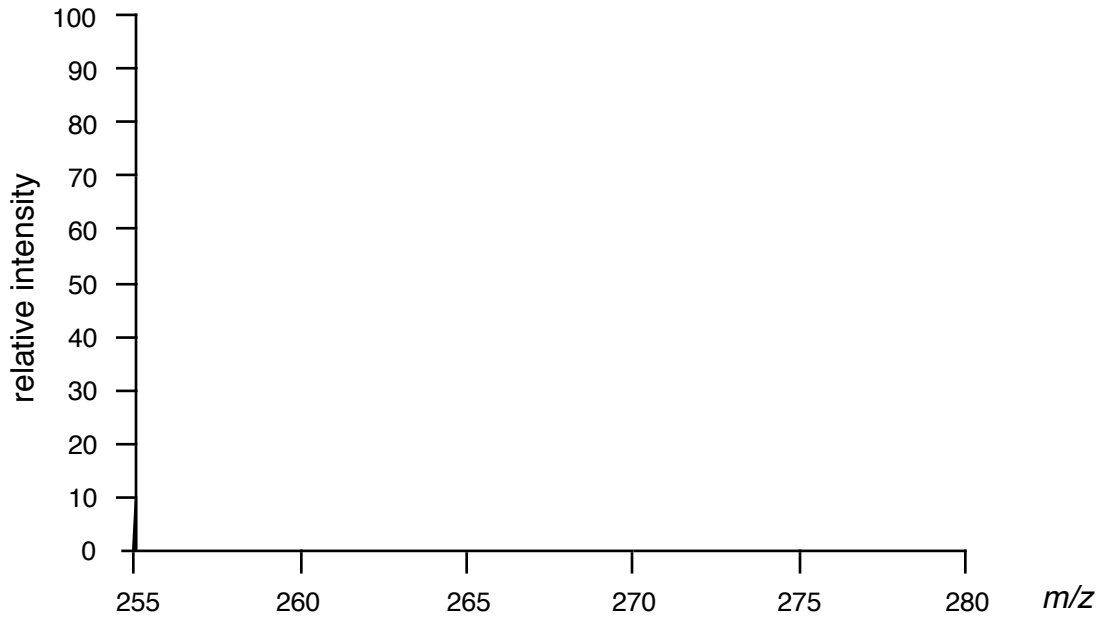
Name _____

b) (20 points) Draw a tree coupling diagram (split forks) and the corresponding ^{1}H NMR signal for proton H_a of diastereomer **1a** in question 3a above.

Tree diagram:

^{1}H NMR signal: _____

c) (10 points) Mass spectrometry: Sketch the isotopic pattern for the parent ion (M^+) of a compound with formula $C_5H_5Br_2NO_2$:

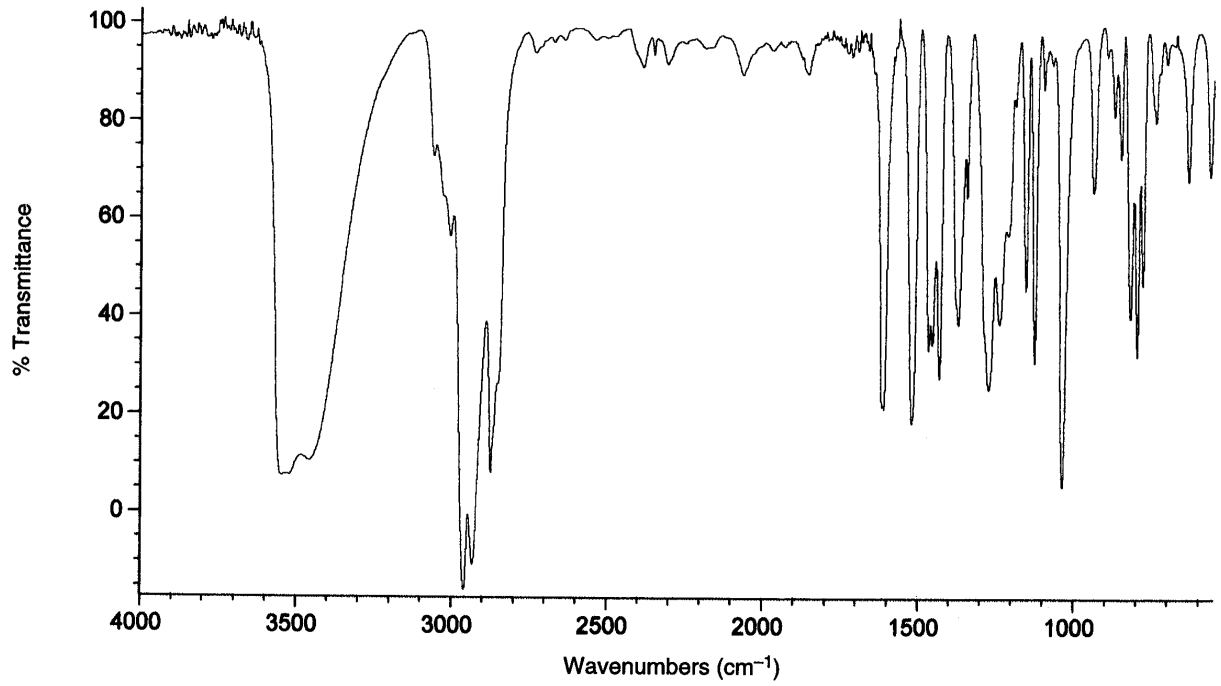


Name _____

4. (40 points) A compound has the molecular formula $C_{10}H_{14}O_2$. Deduce its structure from the IR, ^1H NMR, ^{13}C NMR, 2D-COSY and 2D HMQC spectra shown below. You must provide peak assignments in all spectra to get maximum credit.

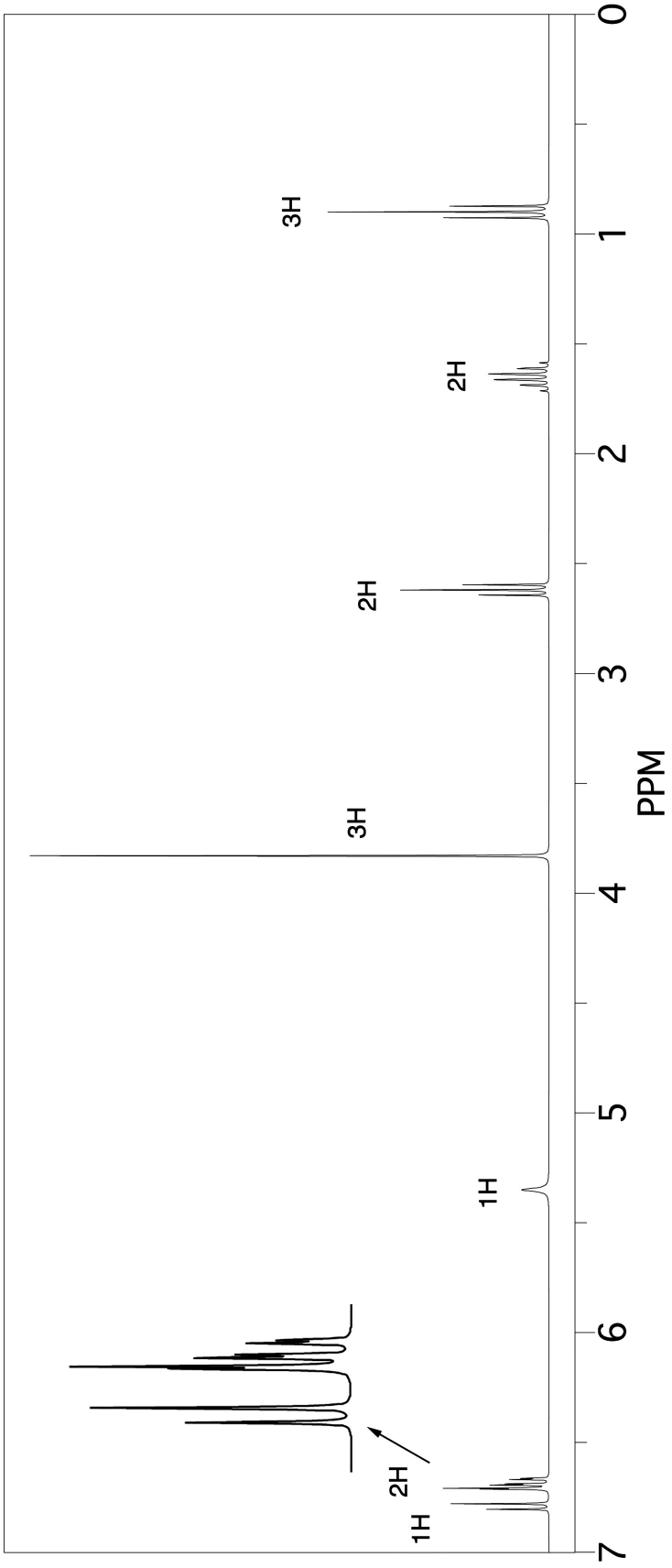
Draw the structure in the space below: Degree of unsaturation: _____

INFRARED



Name

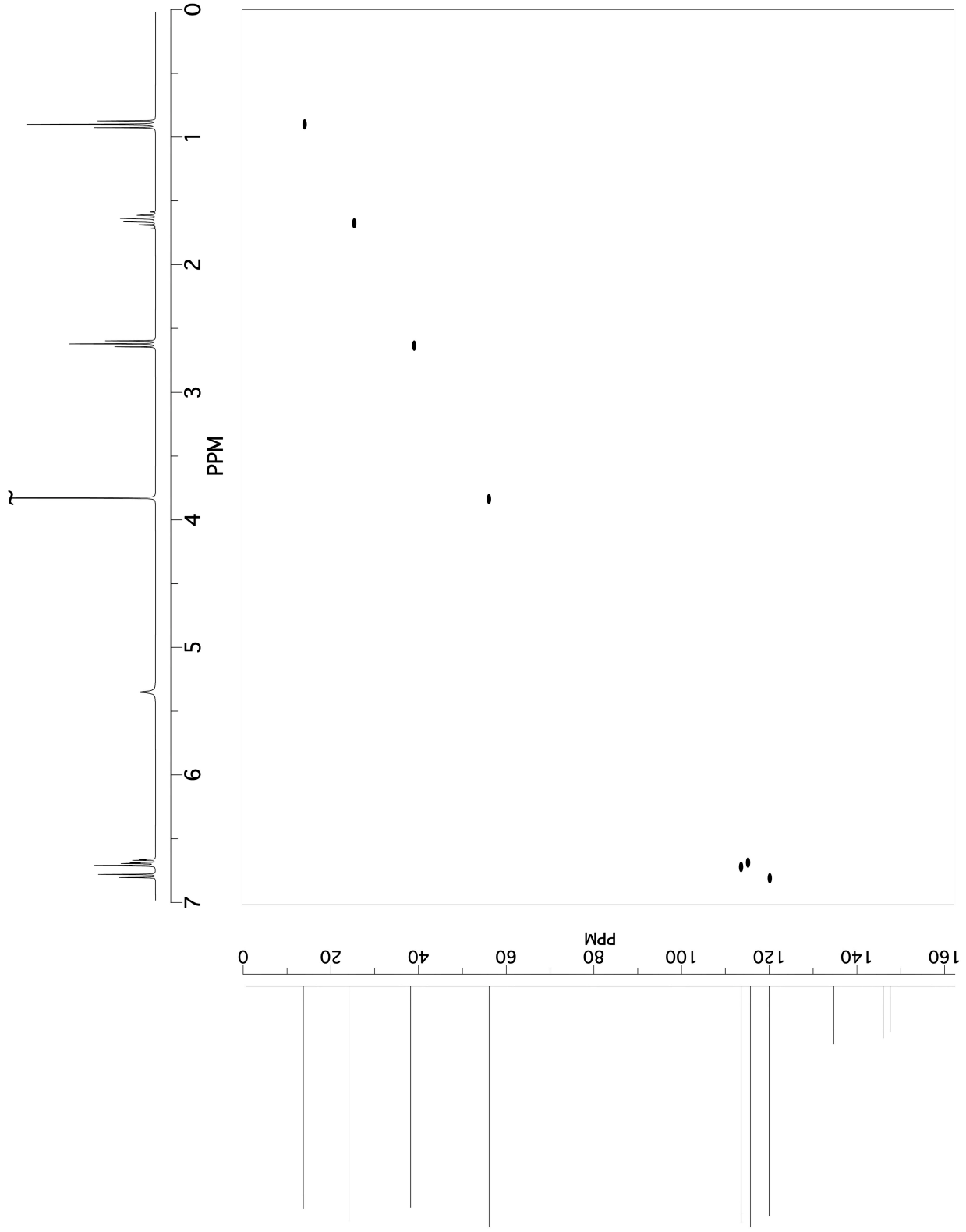
^{1}H NMR spectrum for (**show your structure also here and assign each peak**). Also provide the standard abbreviated **multiplicity** for each signal, e.g. *"d"*:



Please draw structure here and provide assignments between protons on structure and relevant peaks using arrows or letters

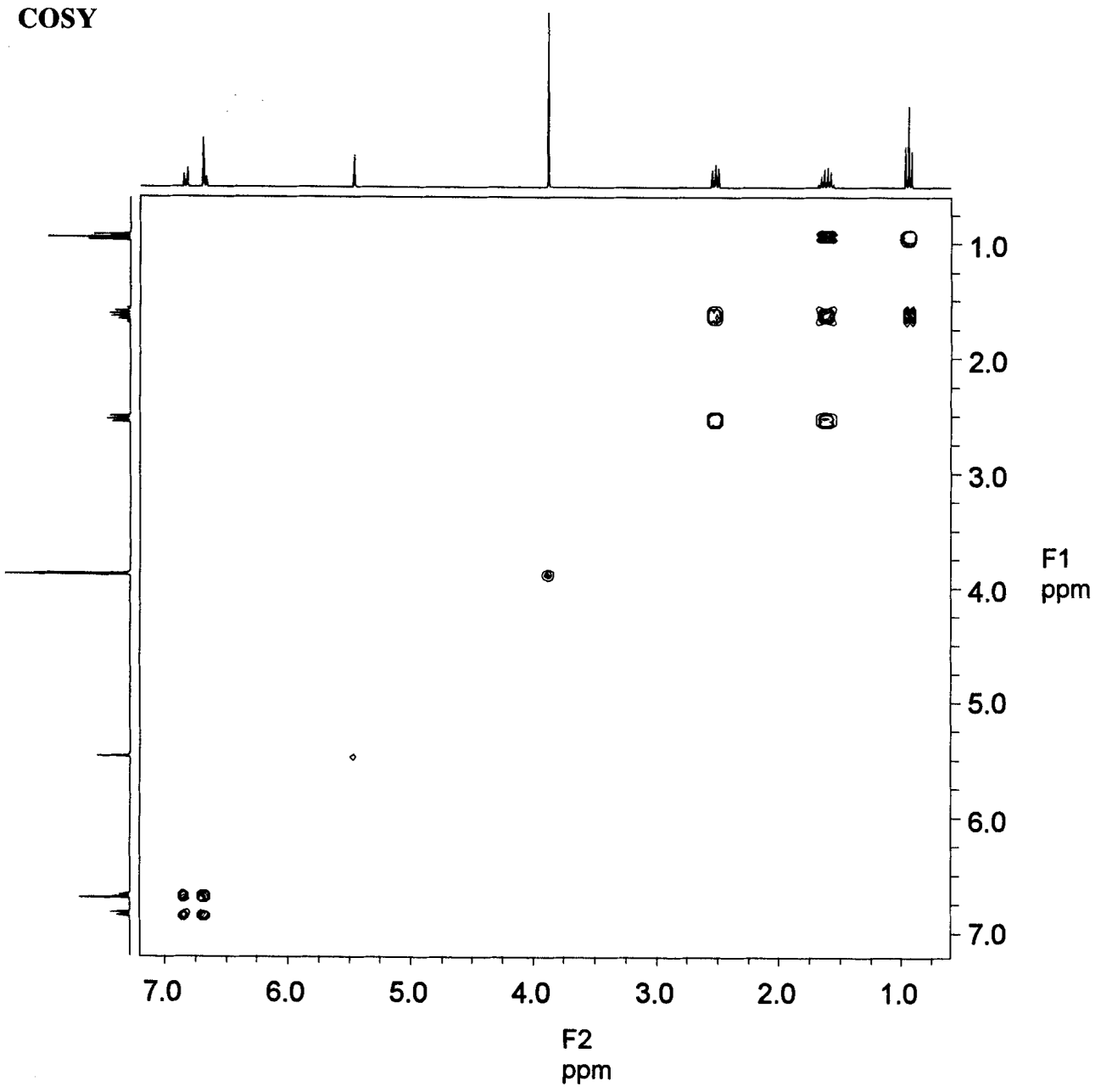
Name

2D HMQC spectrum for question 4 (**show your structure also here and assign each ^{13}C peak that is correlated with protons**):



Name _____

2D COSY NMR spectrum for question 4:



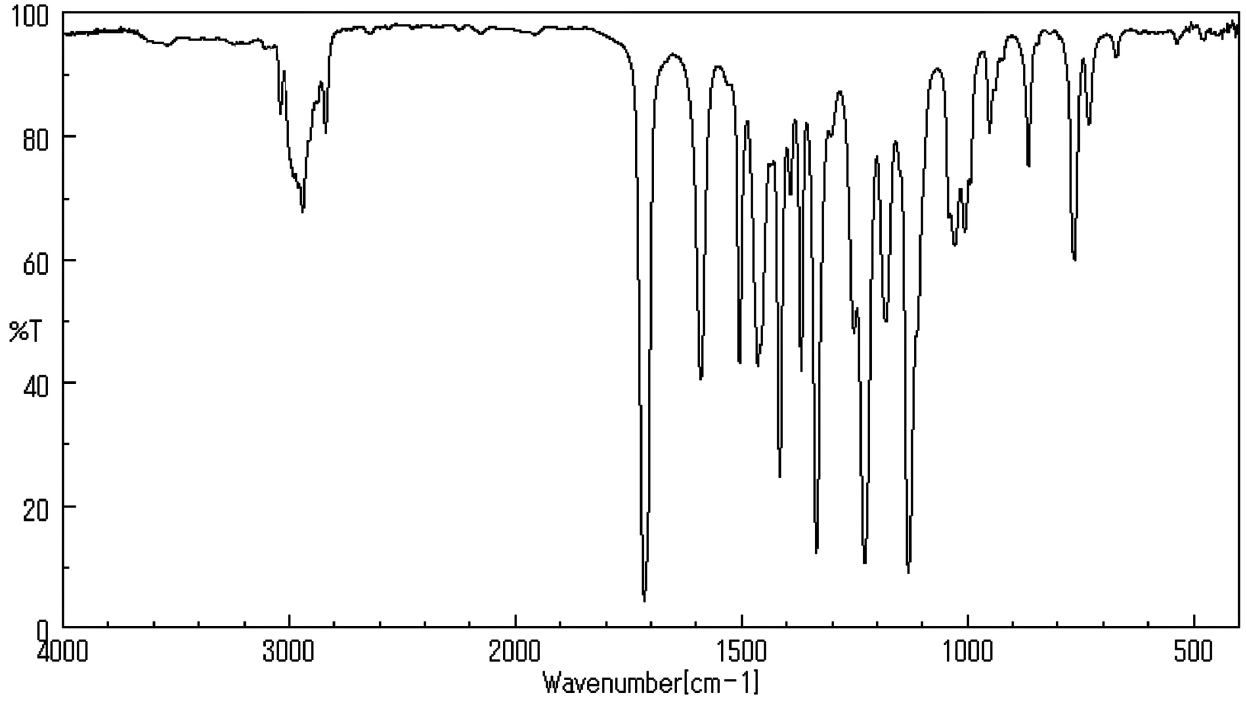
Note: Irradiation of the peak at 3.8 ppm gives strong NOE enhancements for the peaks at 5.5 and 6.7 ppm.

Name _____

5. (50 points) A compound has the molecular formula $C_{12}H_{16}O_5$. Deduce its structure from the IR, ^1H NMR, and ^{13}C NMR spectra given below. You must provide peak assignments in all spectra to get maximum credit.

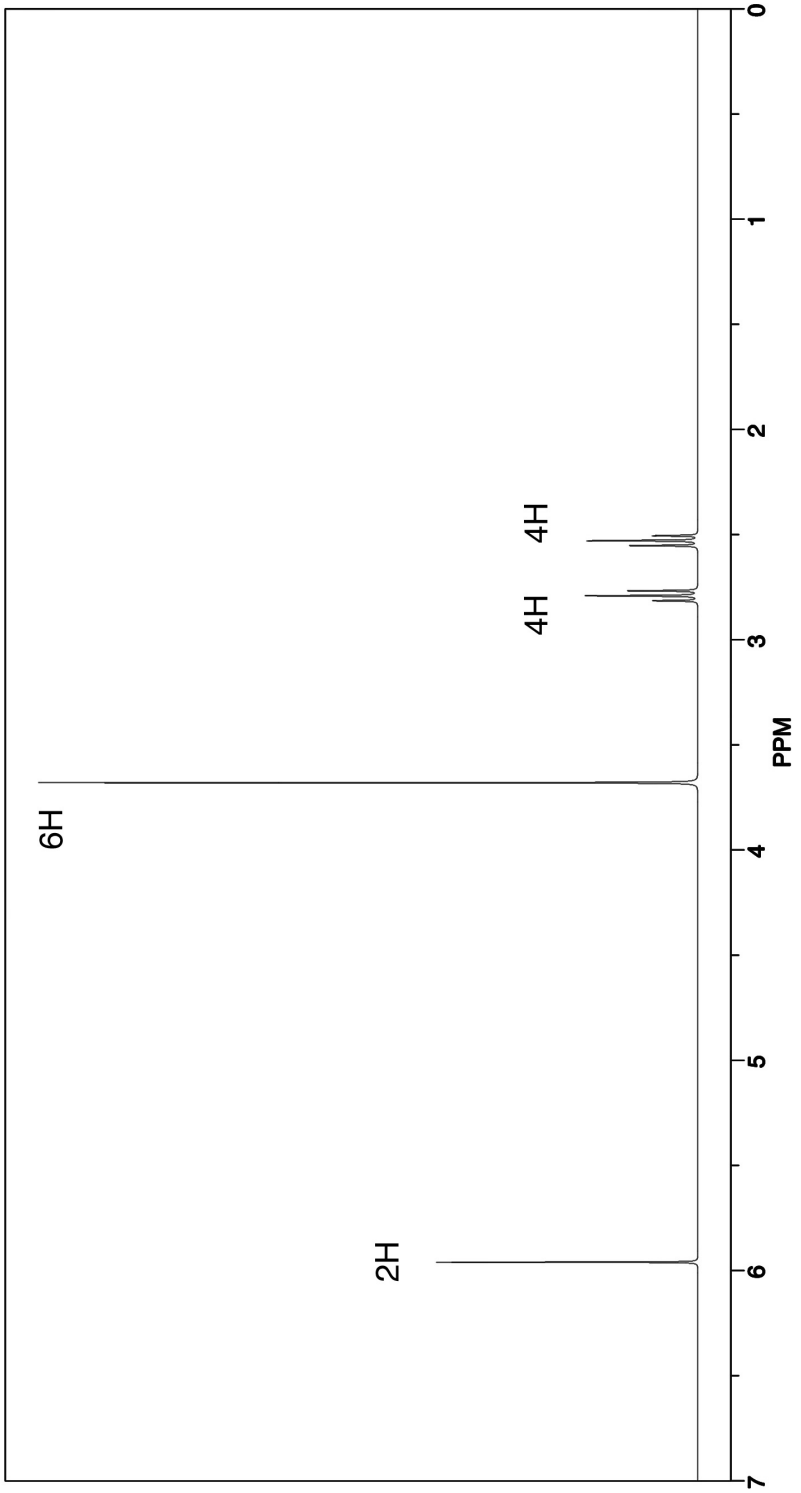
Draw the structure in the space below: Degree of unsaturation: _____

IR spectrum (liquid film):



Name

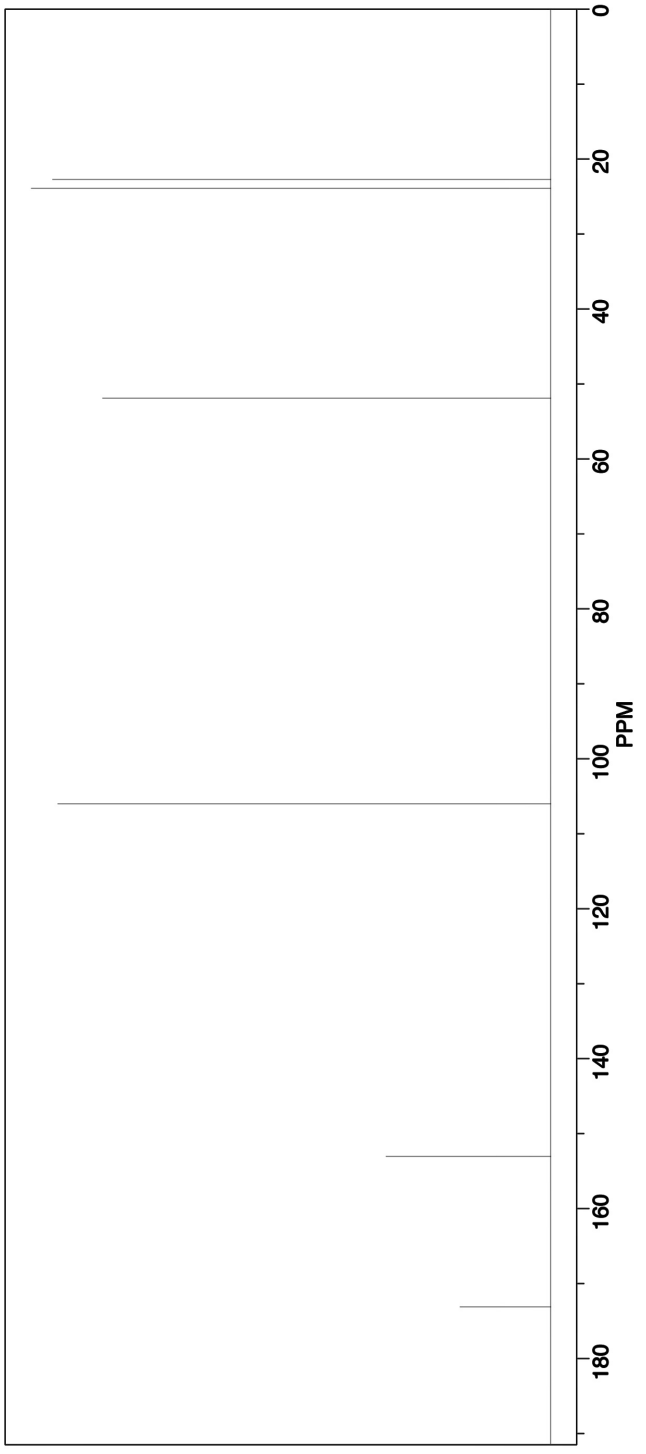
^{1}H NMR spectrum for question 5 (**show your structure also here and assign each peak**). Also provide the standard abbreviated **multiplicity** for each signal, e.g. *"d"*:



Name

^{13}C NMR spectrum for question 5 (**show your structure also here, and assign each peak!**)

Show also a resonance structure that explains the large difference of chemical shifts between the signals at 106 and 153 ppm, supported by a short explanation:



Name

6. (20 points) Assign all the carbons in the ^{13}C NMR spectrum of the compound below using its 2D INADEQUATE spectrum:

Structure: