

Chemistry 210
“Organic Chemistry I”
Fall Semester 2000
Dr. Rainer Glaser

Examination #4
“H-NMR Spectroscopy”

Friday, December 8, 2000, 9:00 - 9:30

Name:

Answer Key

Question 1. NMR Basics.	20	
Question 2. H-NMR Spectrum Interpretation.	15	
Question 3. H-NMR Spectrum Prediction.	15	
Total	50	

Question 1. NMR Basics. (20 points)

(a) What does “NMR” stand for? Nuclear Magnetic Resonance. (3 p.)

(b) What kind of radiation is used to afford the flipping of the nuclear spins? (2 p.)

(1) microwaves (2) **radiowaves** (3) gamma rays (4) infrared light

(c) H-atoms with higher chemical shift absorb radiation of _____ (**higher**, lower) frequency. (2 p.)

(d) Chemical shifts are relative values that are independent of the magnetic field strength of the NMR spectrometer. The chemical shift values are given relative to “TMS”. Draw the structure of TMS, provide the full name of TMS, and specify the exact chemical shift of TMS. (3 p.)

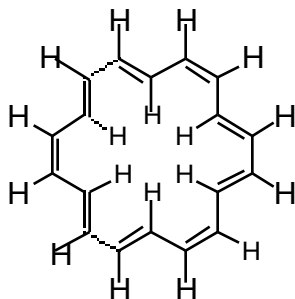
Si(CH₃)₄
Tetramethylsilane
δ = 0 ppm

(e) An H-atom is said to be “deshielded” when the H-atom is _____ (**positively**, negatively) charged and such “deshielded” H-atoms show _____ (**high**, low) chemical shifts. (4 p.)

(f) Which class of compounds contains the H-atom with the highest chemical shift? (2 p.)

(1) alcohols (2) amines (3) **carboxylic acids** (4) esters

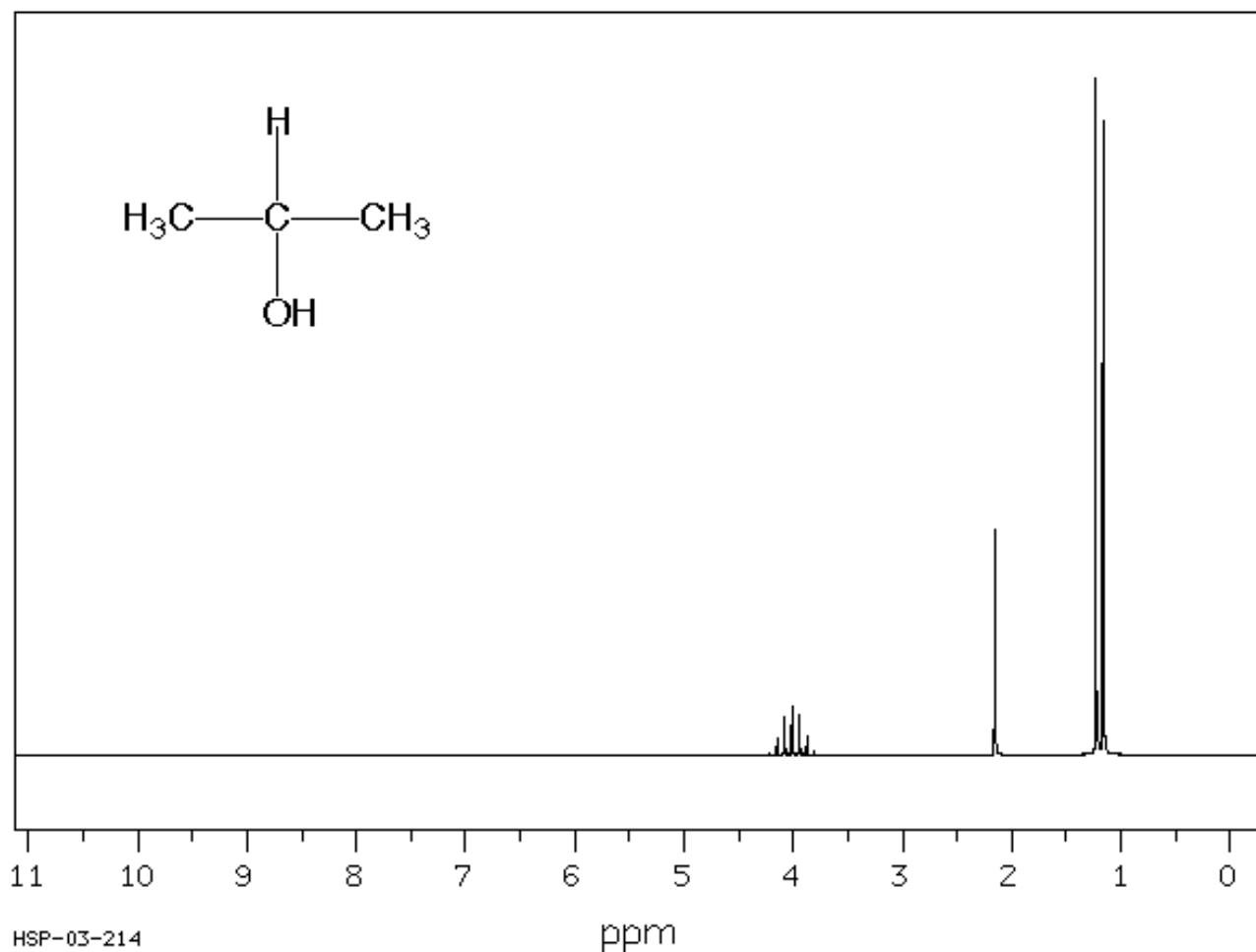
(g) [18]-Annulene is shown. This molecule is featured in the **Visualization Center** that accompanies the NMR chapter. The ring current in the π-clouds of this aromatic system _____ (**enhances**, diminishes) the external magnetic field outside of the ring and _____ (**high**, low) chemical shifts are found for the H-atoms on the outside of the rings. On the other hand, the H-atoms in the center experience _____ (enhanced, **reduced**) effective magnetic fields. (4 points)



[18]-Annulene

Question 2. H-NMR Spectrum Interpretation. (15 points)

The H-NMR Spectrum of 2-Propanol.



Assign the H-NMR Spectrum of 2-propanol.

For each peak, write next to the peak what kind of splitting pattern the peaks shows (singlet etc.).

For each peak, write next to the peak how many H-atoms cause the peak (1H, 2H, etc.).

For each peak, write next to the peak which (group of) H-atom(s) causes the peak.

For the signal at 4 ppm, what line intensities would you expect in the ideal case (use Pascal triangle)?

Above 1ppm: doublet, 6H, two methyl groups, coupled to unique CH.

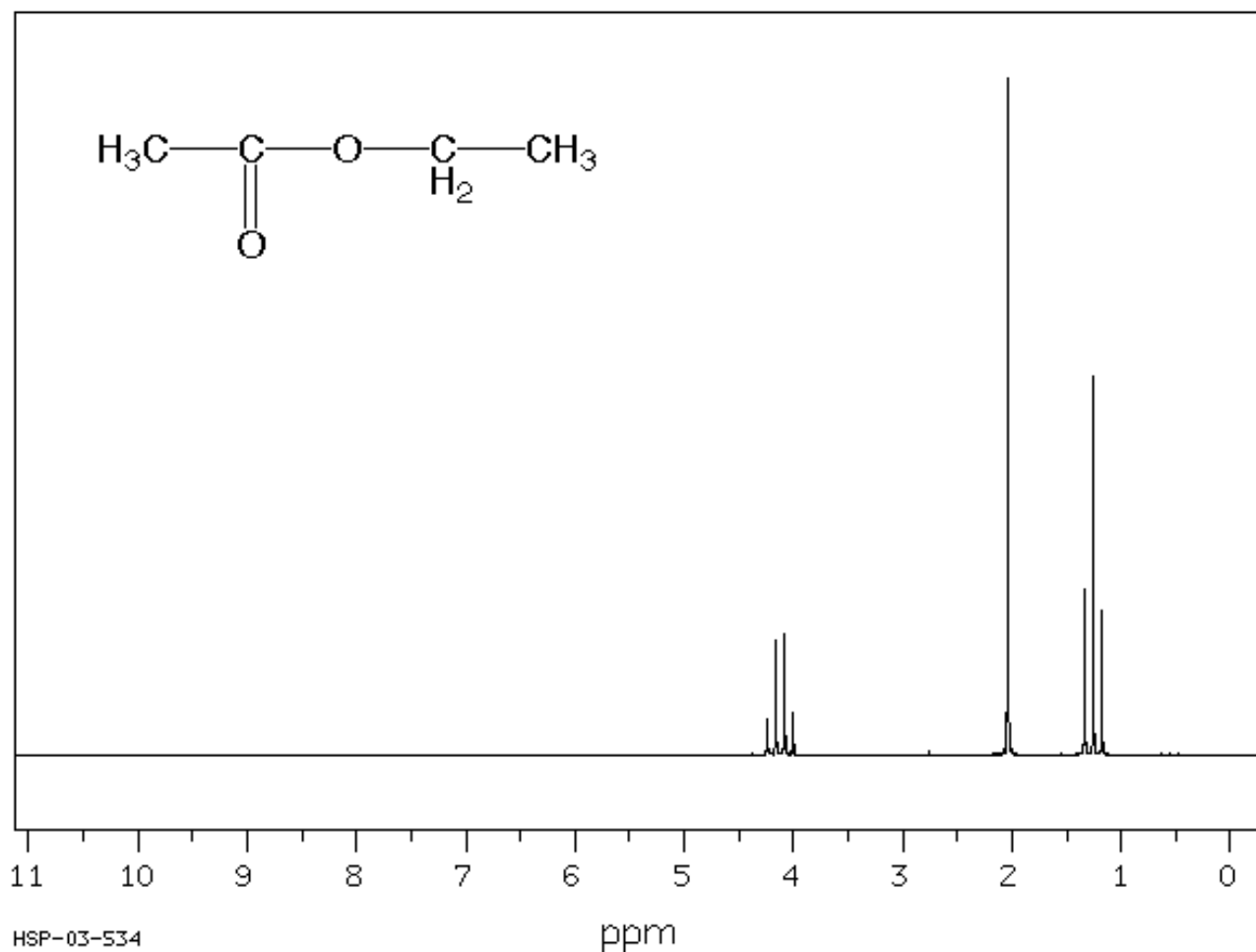
At 4ppm: Septet, 1H, unique CHm coupled to six equivalent neighbors.

Above 2ppm: Singlet, 1H, the alcohol, does not couple (exchange).

The line intensities of the septet: 1 : 6 : 15 : 20 : 15 : 6 : 1

Question 3. H-NMR Spectrum Prediction. (15 points)

The H-NMR Spectrum of Ethyl Acetate.



Predict the H-NMR Spectrum of Ethyl Acetate.

Predict the number of peaks. **3 peaks**

Predict the approximate chemical shifts of all peaks using the chemical shift tables.

Ethyl group: Methylene much more deshielded than methyl.

The methyl on the carbonyl side is deshielded less than the methylene on the O-side.

Predict the splitting patterns of all peaks.

The acetic acid methyl group is a singlet.

The ethyl groups gives a quartet (CH_2) and a triplet (CH_3).

Draw an approximate spectrum in the above template. The spectrum should reflect chemical shifts, signal intensities and splitting due to spin-spin coupling.