

name: _____ (please print) signature: _____

honor pledge: I will neither give nor receive unauthorized information while taking this exam.

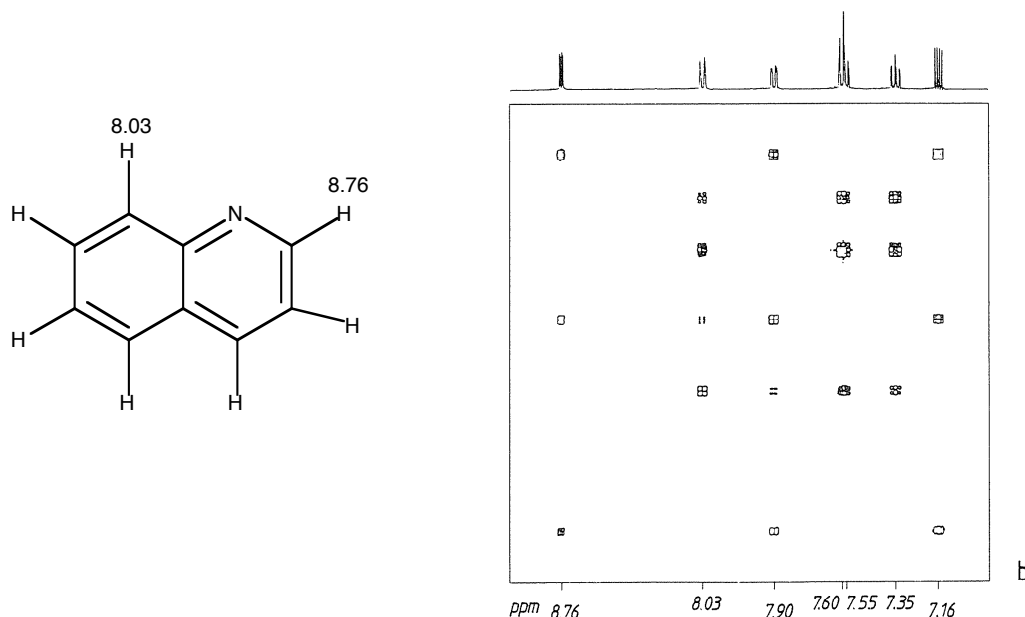
(1a) (5 pts) What advantages does DEPT have over off-resonance ^{13}C -NMR spectroscopy for giving CH multiplicities?

(1b) (5 pts) What information is gained from a CH COSY (HETCOR) which is not obtained from DEPT?

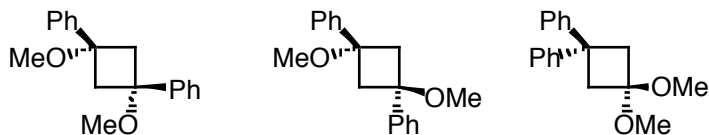
(1c) (5 pts) Write a structure that will have both $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ absorptions and indicate which will be at longest wavelength.

(1d) (5 pts) List five ionization methods used in mass spectrometry.

(1e) (10 pts) Use the following COSY spectrum to assign the proton resonances of quinoline. Please write the δ -value next to the appropriate H in the structure. Two assignments are made for you.



(1f) (5 pts) Describe how you could use ^{13}C - and ^1H -NMR to distinguish the following isomers without worrying about chemical shift differences?



(2) (40 pts) Consider the following spectra for compd **1** (handout) and answer the following questions on this page. Finally, proceed to assign all peaks in the ^1H -NMR and ^{13}C -NMR spectra (on the spectra) to the extent possible.

(a) (2 pts) What is the mol. wt. for compd **1**?

(b) (3 pts) Give 3 possible formulae (with associated UI) for this structure:

(c) (2 pts) What is learned about the structure from the IR spectrum?

(d) (5 pts) Based on the NMR data, pick a "best formula" for this structure and indicate why it is best.

(e) (8 pts) Provide the structural fragments that gives rise to the following signals:

(^1H -NMR) 2H quartet at 4.15 ppm =

(^1H -NMR) 3H doublet at 1.8 ppm =

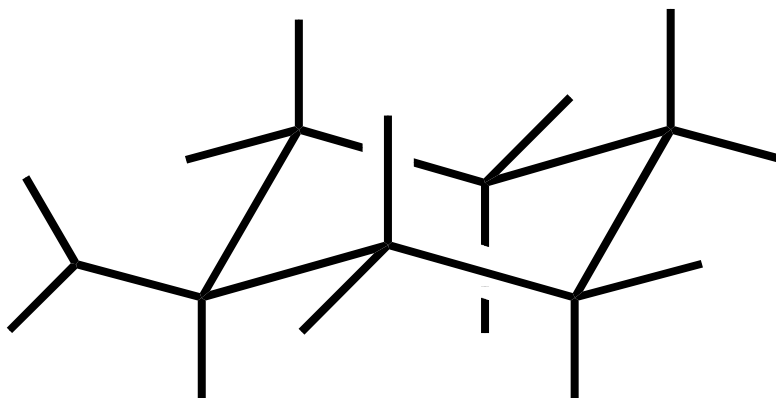
(COSY) coupled spin systems present in the molecule =

(f) (5 pts) Provide the structure and indicate stereochemistry and how it is determined.

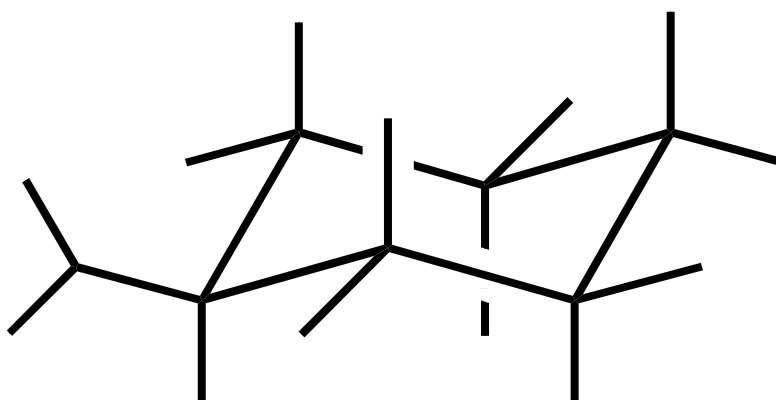
(g) (15 pts) Assign ^1H -NMR and ^{13}C -NMR signals (on the spectra in the handout).

(3) (25 pts) Work Problem #33 (handout). Use the large chair structure below for compd 4 and add all the groups (including Hs) attached to the ring and assign all proton shifts by writing the chemical shifts on your structure. The isopropyl group is already shown. Place the CO₂H group at the next position (coming out of the page) in the appropriate position (axial or equatorial). Use the second chair structure to label the chemical shifts of the carbons. The proton and carbon chemical shift positions are listed on the HH COSY and CH COSY data, respectively.

for labeling proton resonances



for labeling carbon resonances



scratch