Massachusetts Institute of Technology
Organic Chemistry 5.13

Friday, September 30, 2005 Prof. Timothy F. Jamison

Hour Exam #1

Name SOLUTIONS

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

Official 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.

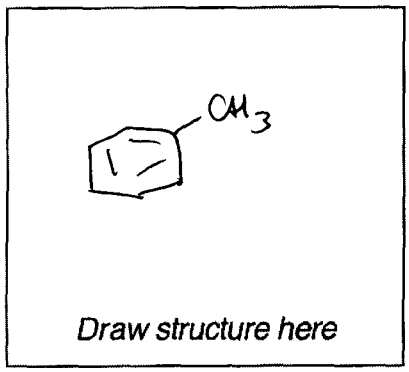
You should have **11** pages total: **6** exam pages including this page, **3** pages of reference information, and **2** blank pages for scratchwork.

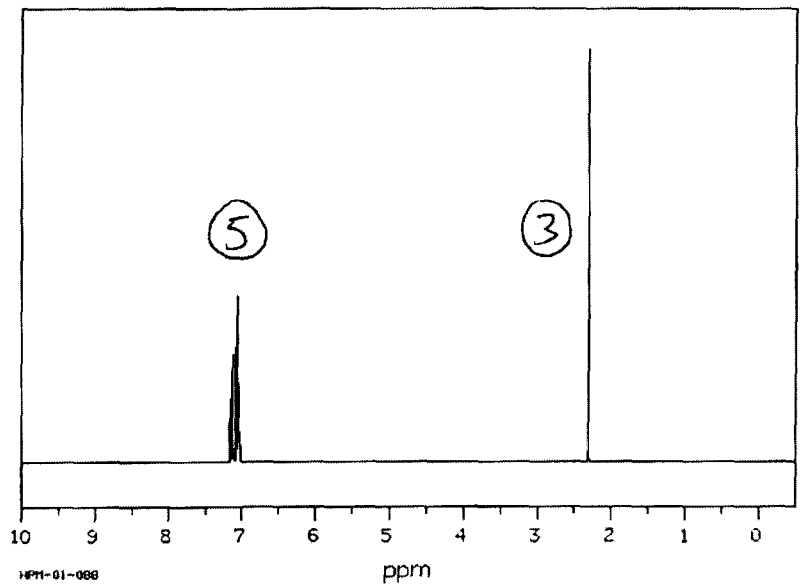
Question:		**Grader:**
1. _____/	**40 points**	_____
2. _____/	**30 points**	_____
3. _____/	**30 points**	_____
Total: _____/	**100 points**	_____

1. **(40 points total – 5 points each)** The molecular formulas and ^{1}H NMR spectra of **8 common organic solvents** are provided below and on the following 2 pages. For each, neatly **draw the entire structure** (i.e., not the acronym) in the box provided. In some cases, relative integration values (circled numbers) and/or other information have been provided.

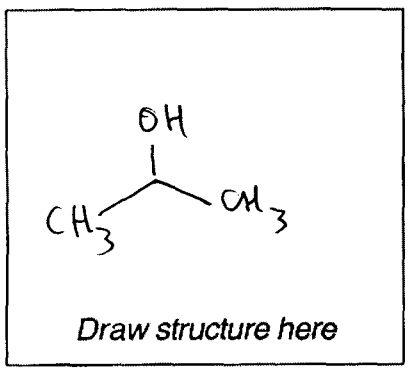
Note: Do **not** represent functional groups with partial molecular formulas or other abbreviations. For example, do not use "Ph" or "C_6H_5" for a phenyl group. **Draw** the entire group (including hydrogen atoms).

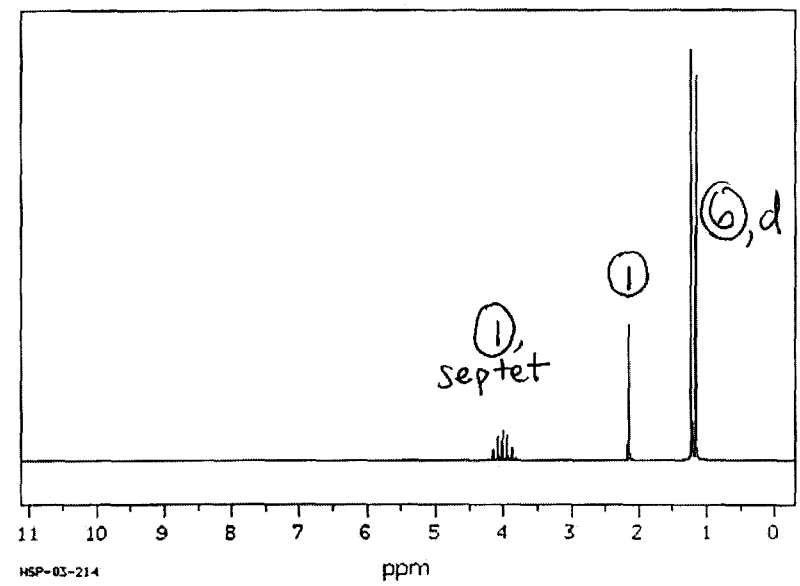
a. C_7H_8



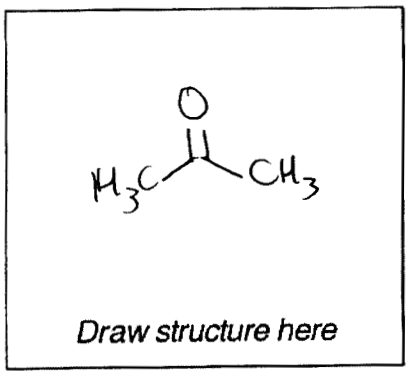


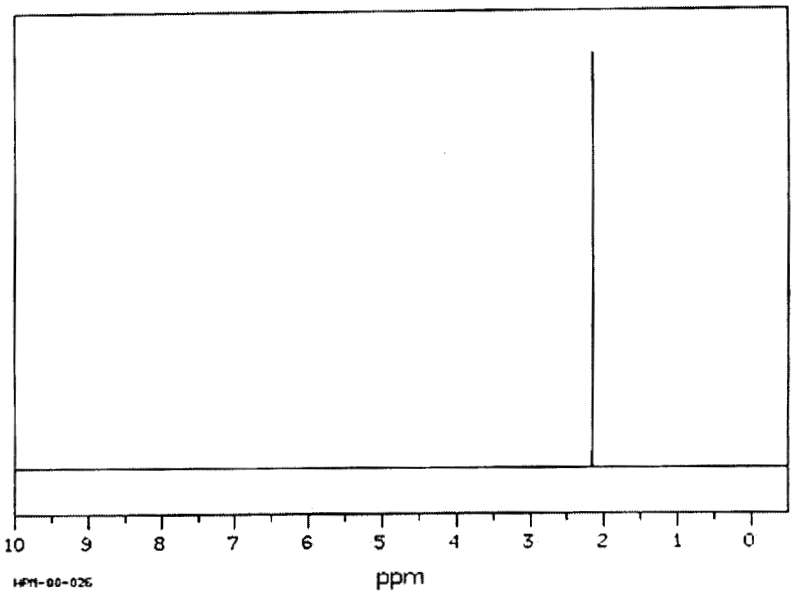
b. C_3H_8O



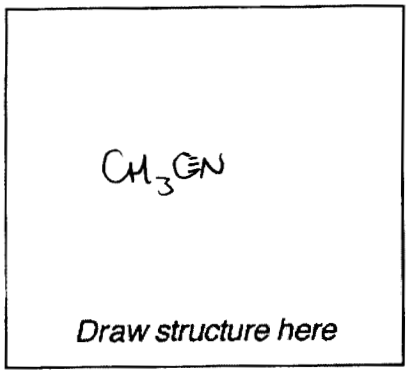


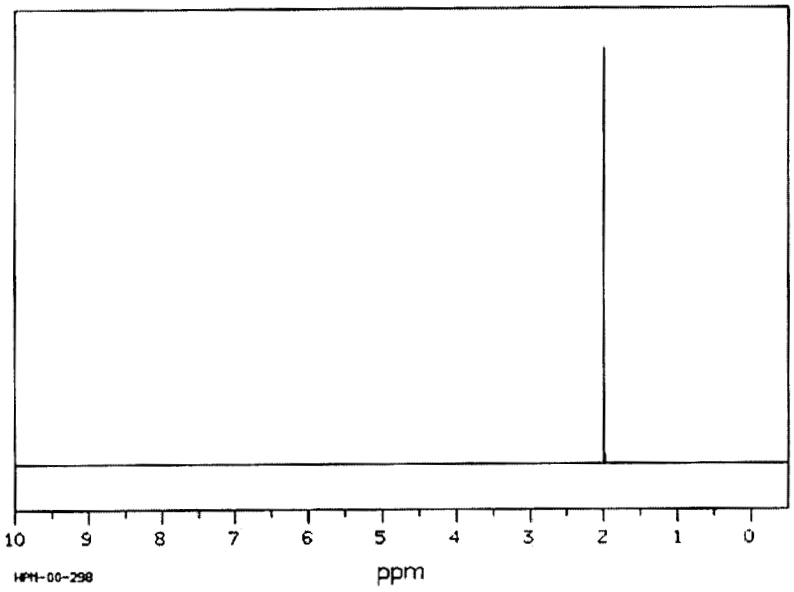
c. C_3H_6O



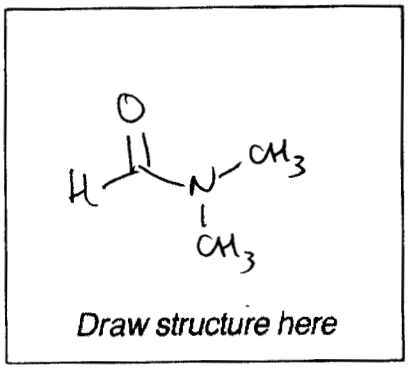


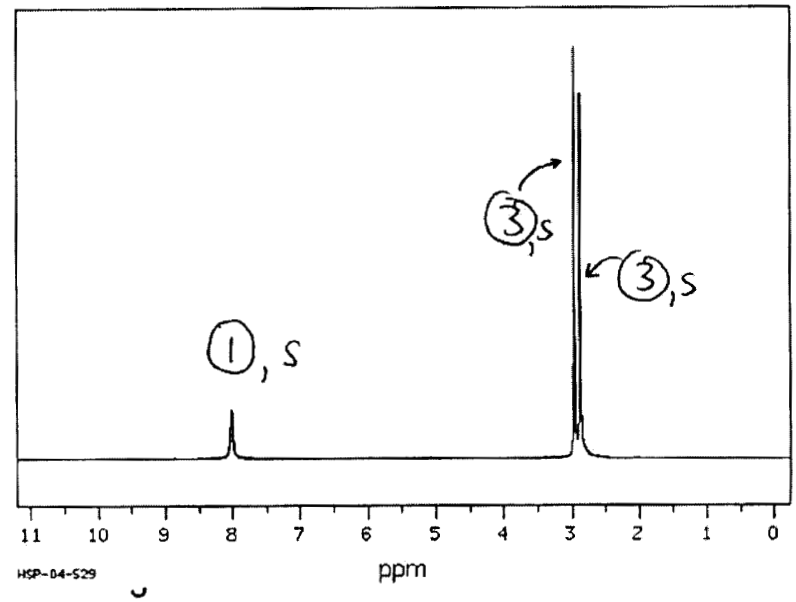
d. C_2H_3N



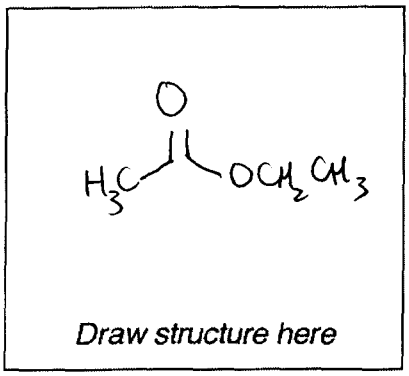


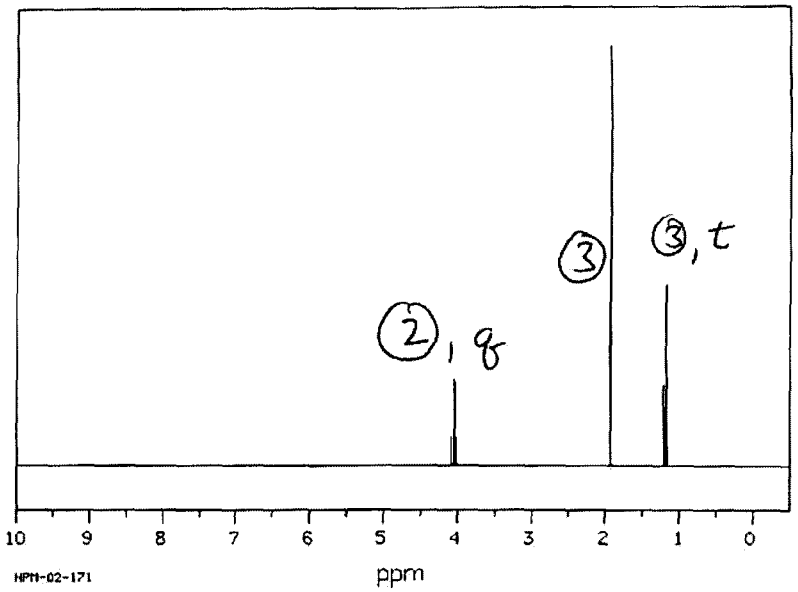
e. C_3H_7NO



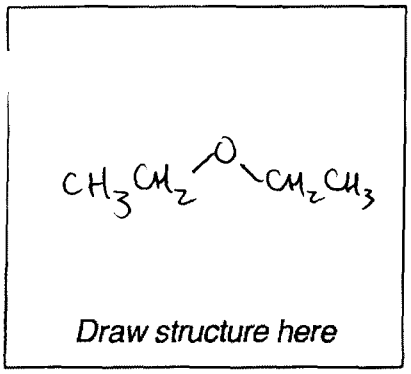


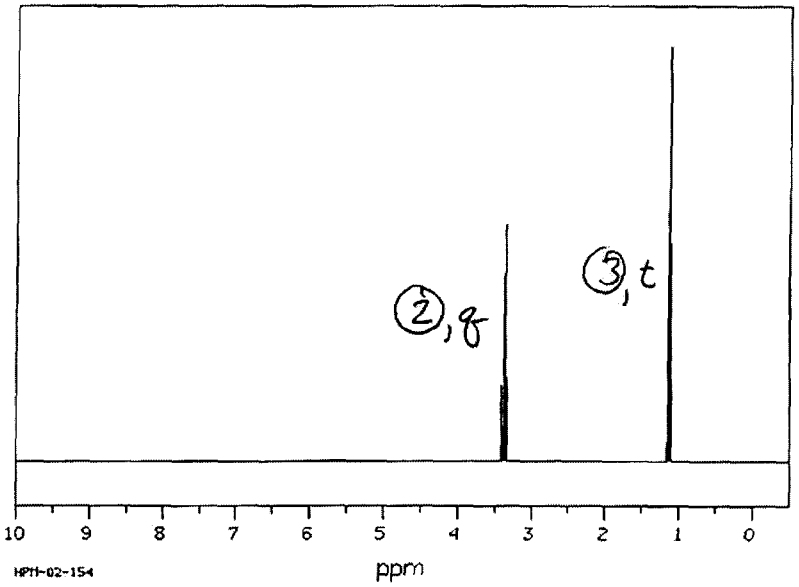
f. $C_4H_8O_2$



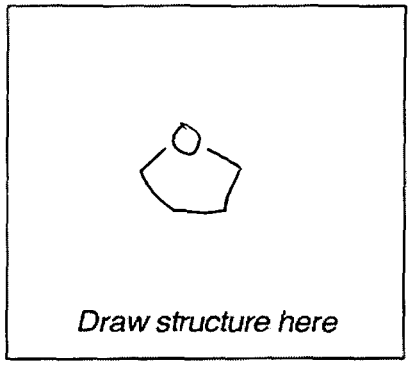


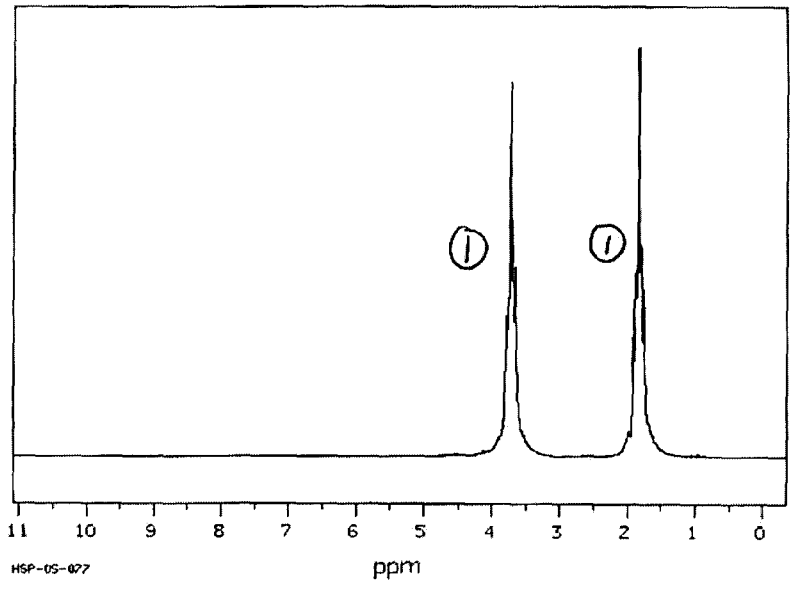
g. $C_4H_{10}O$





h. C_4H_8O





2. **(30 points total)** Answer the questions below about the structure that has the following data:

EA	C, 81.61; H, 11.06; N, 7.32
MS	191, 176.
^{13}C NMR	162.7, 136.5, 118.9, 35.1, 31.9
^{1}H NMR	7.59 (t, J = 7.8, 1H), 7.14 (d, J = 7.8, 2H), 1.34 (s, 18H)

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

$C_{13}H_{21}N$

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

$13 - \frac{21}{2} + \frac{1}{2} + 1 = 4$

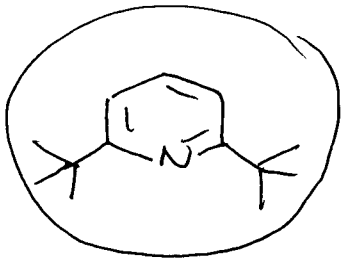
c. (2 points) How many "types of carbon" (chemically non-equivalent) does this compound have? **Circle** your final answer.

5

d. (3 points) How many "types of hydrogen" (chemically non-equivalent) does this compound have? **Circle** your final answer.

3

e. (10 points) **In the space below, draw the structure of the molecule that is consistent with all of the data provided**. **Circle** your final answer.



3. **(30 points total)** Answer the questions below about the structure that has the following data:

EA	C, 75.69; H, 8.80
M^+	206
IR	3430 (broad), 1705 (strong)
^{13}C NMR	181.4, 140.9, 137.0, 129.5, 127.4, 45.9, 44.1, 30.3, 22.5, 18.2
^1H NMR	11.9 (broad s, 1H), 7.21 (d, J = 7.7, 2H), 7.09 (d, J = 7.7, 2H), 3.70 (q, J = 7.0, 1H), 2.44 (d, J = 6.8, 2H), 1.84 (nonet (9 lines), J = 6.8, 1H), 1.49 (d, J = 7.0, 3H), 0.89 (d, J = 6.8, 6H)

a. (7 points) Determine the **molecular** formula. **Circle** your final answer.

$C_{13}H_{18}O_2$

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

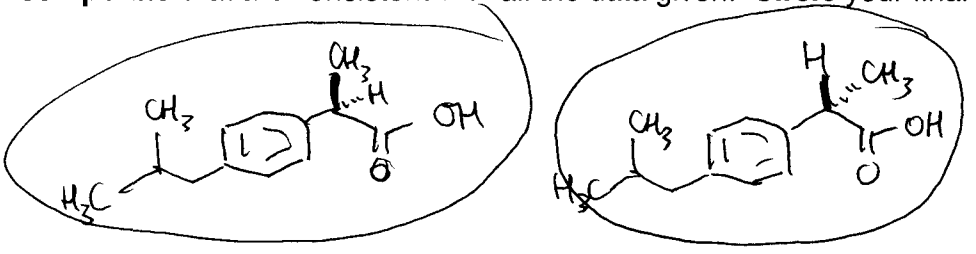
$13 - \frac{18}{2} + 1 = 5$

c. (8 points) Which protons are coupled to which? Complete the tables below using the NMR data above. Write H1, H2, etc. or "none", as appropriate, in the box provided, and list **all protons** to which a given proton is coupled.

Proton(s)	∂ (ppm)	Coupled to
H1	11.9	none
H2	7.21	H3
H3	7.09	H2
H4	3.70	H7

Proton(s)	∂ (ppm)	Coupled to
H5	2.44	H6
H6	1.84	H5, H8
H7	1.49	H4
H8	0.89	H6

d. (10 points) Draw **all** of the possible **enantiomers and diastereomers of the unknown compound** that are consistent with all the data given. **Circle** your final answers.



e. (**Extra credit** – 5 points total) What is the common name of this over-the-counter pharmaceutical (3 points), and for which symptoms is it indicated (2 points)?

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