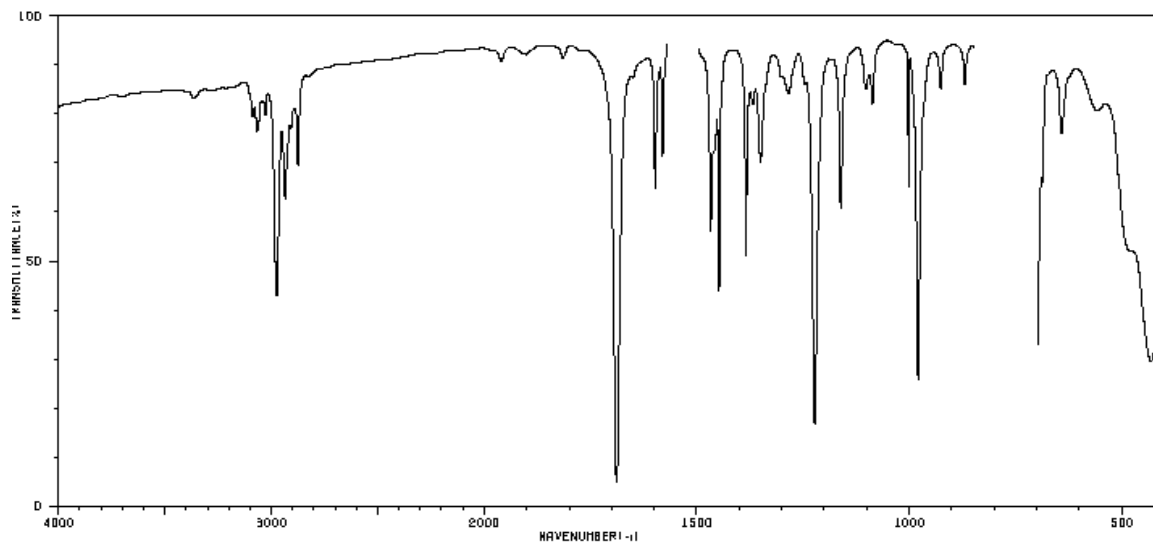
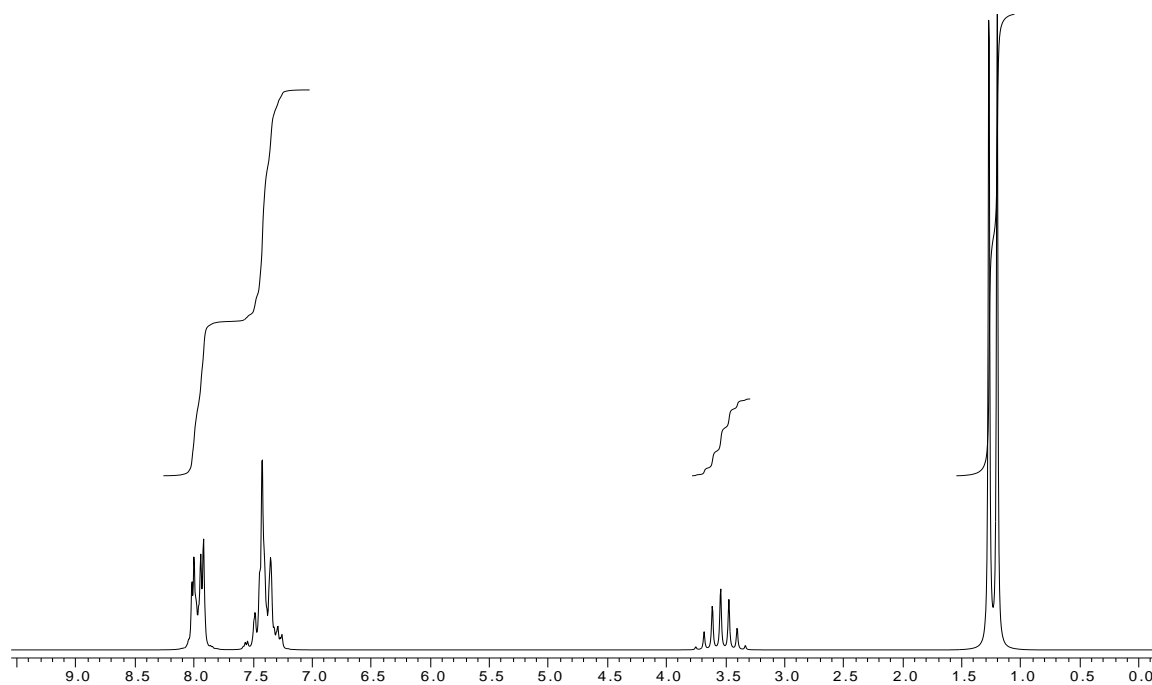


Problem Set 1 – ¹H NMR Spectra

1. The IR and ¹H NMR spectra of a compound of molecular formula C₁₀H₁₂O are given below.



SDBSWeb: <http://www.aist.go.jp/RIODB/SDBS/> (22-12-09)



- a. Calculate the degree of unsaturation.

$$(2 \times 10 - 12 + 2) / 2 = 5$$

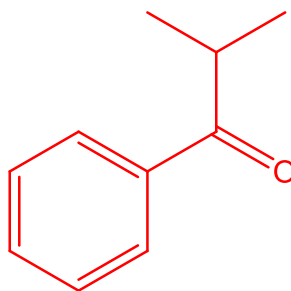
b. List the possible functional groups gleaned from the molecular formula.

Alcohol, aldehyde, ether, ketone, phenol

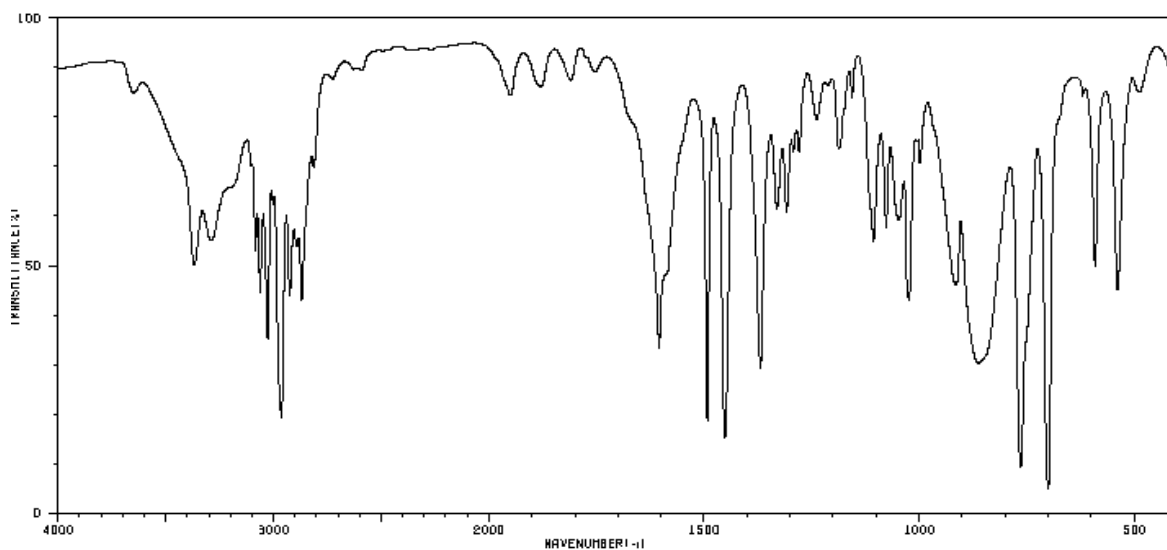
c. What is the oxygen-containing functional group that the IR spectrum shows to be present in the unknown?

Ketone

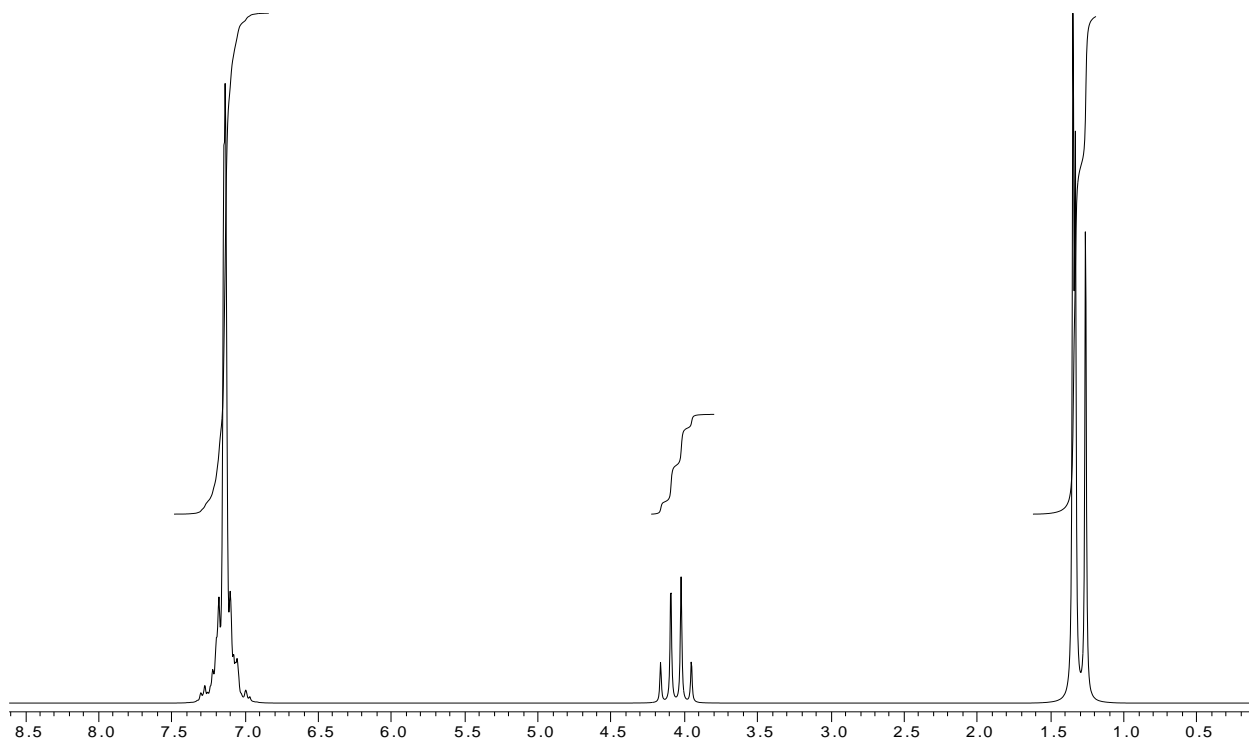
d. Propose a structure for this compound.



2. The IR and ^1H NMR spectra of a compound of molecular formula $\text{C}_8\text{H}_{11}\text{N}$ are given below.



SDBSWeb : <http://riodb01.ibase.aist.go.jp/sdbs/> (National Institute of Advanced Industrial Science and Technology, 27/07/2010)



a. Calculate the degree of unsaturation.

$$(2 \times 8 + 1 - 11 + 2)/2 = 4$$

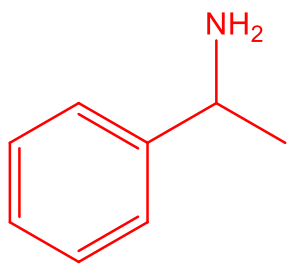
b. List the possible functional groups gleaned from the molecular formula.

Nitrile, primary amine, secondary amine, tertiary amine

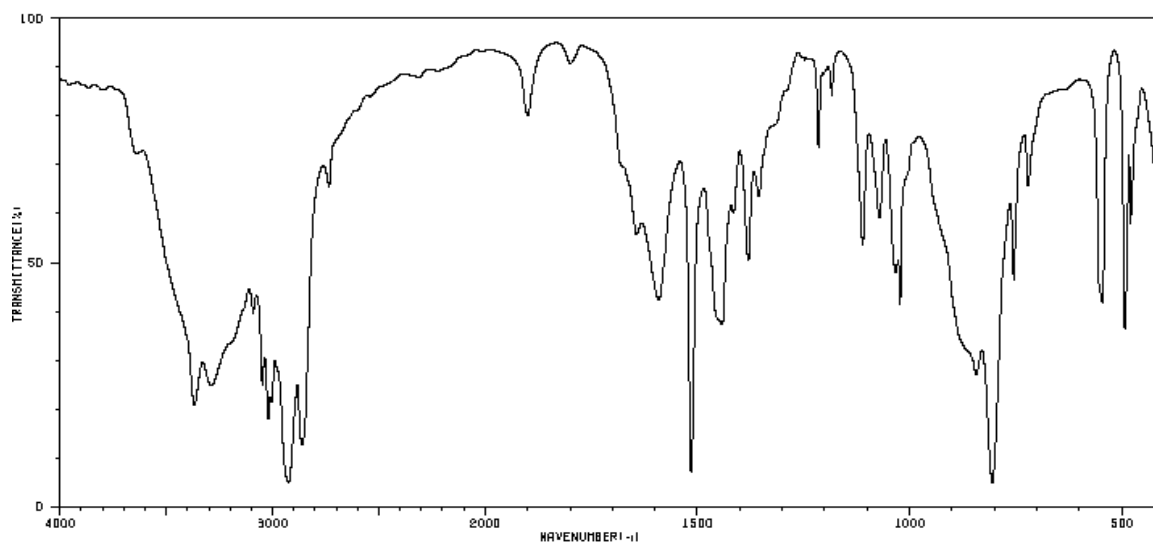
c. What is the nitrogen-containing functional group that the IR spectrum shows to be present in the unknown?

Primary amine

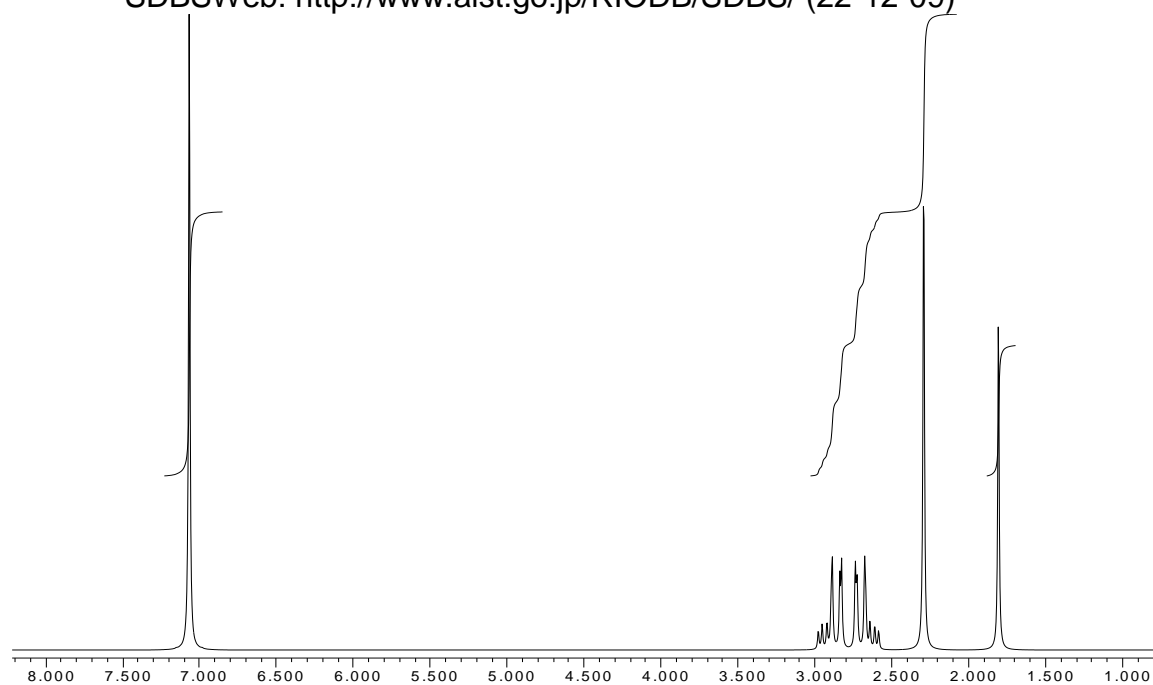
d. Propose a structure for this compound.



3. The IR and ^1H NMR spectra of a compound of molecular formula $\text{C}_9\text{H}_{13}\text{N}$ are given below.



SDBSWeb: <http://www.aist.go.jp/RIODB/SDBS/> (22-12-09)



d. Calculate the degree of unsaturation.

$$(2 \times 9 + 1 - 13 + 2)/2 = 4$$

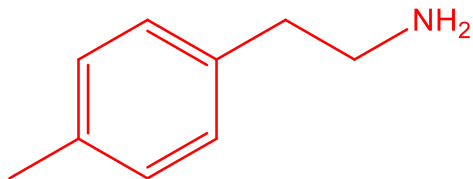
e. List the possible functional groups gleaned from the molecular formula.

Nitrile, primary amine, secondary amine, tertiary amine

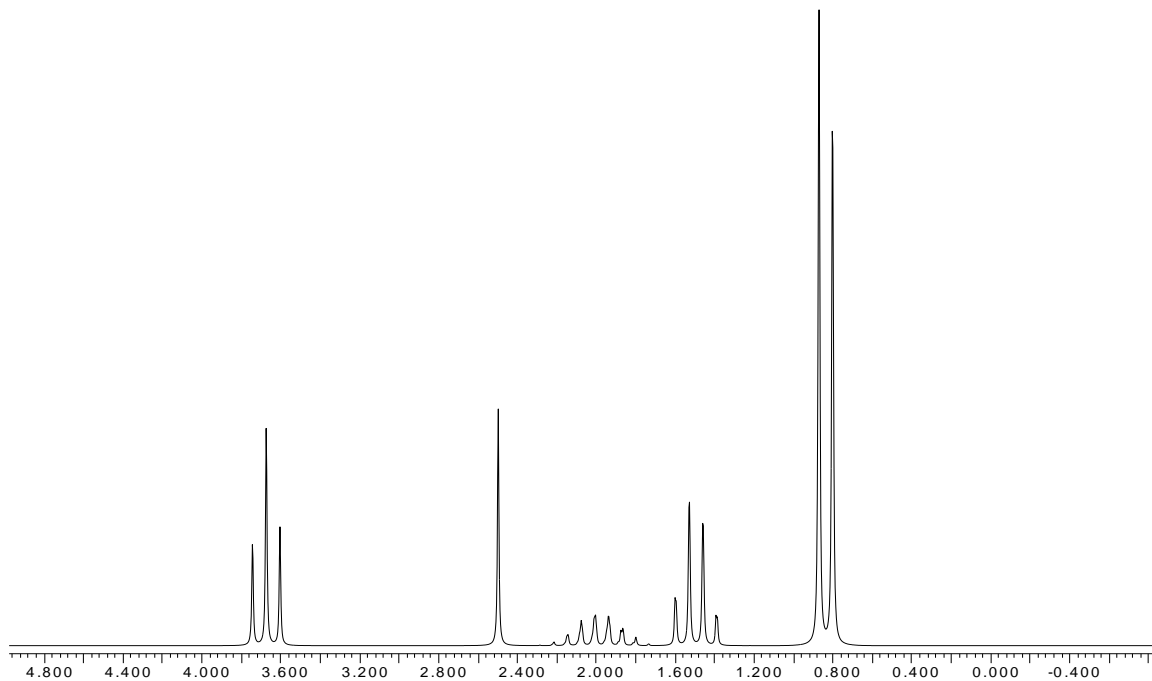
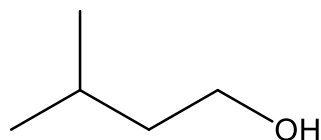
f. What is the nitrogen-containing functional group that the IR spectrum shows to be present in the unknown?

Primary amine

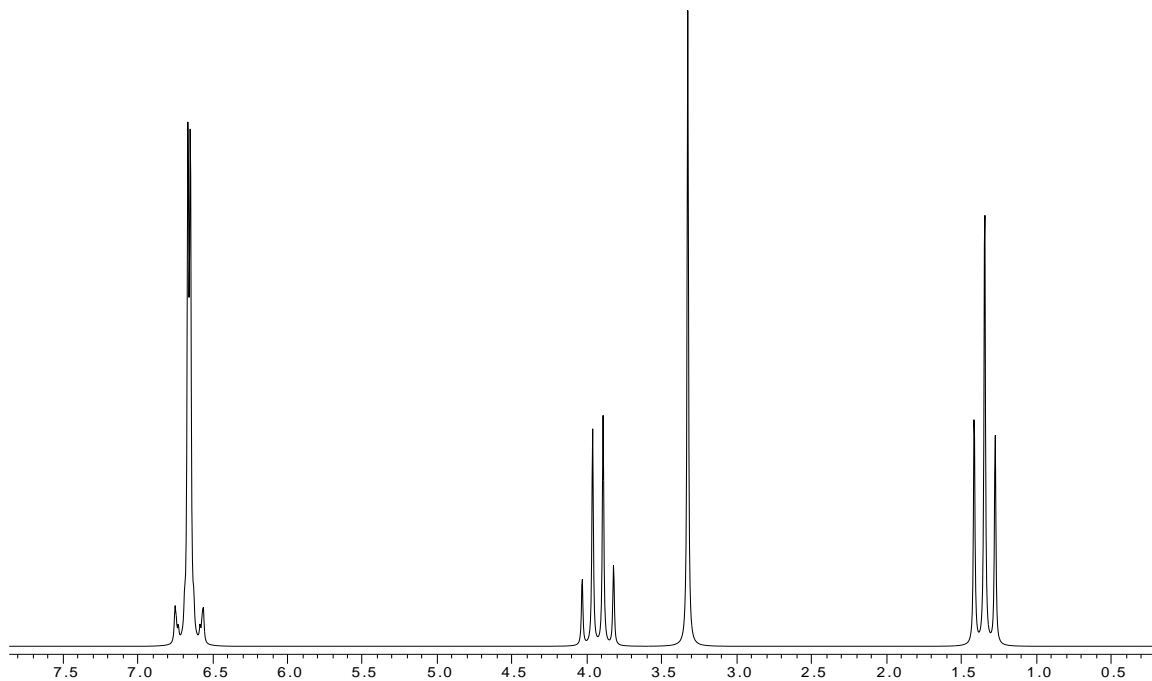
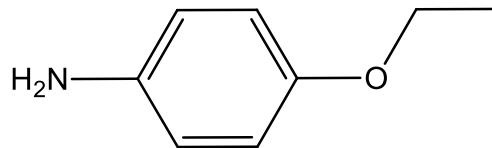
g. Propose a structure for this compound.



4. Sketch the expected ^1H NMR spectrum of the following compound. Pay attention to multiplicity and approximate chemical shifts:

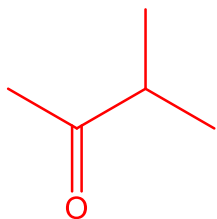


5. Sketch the expected ^1H NMR spectrum of the following compound. Pay attention to multiplicity and approximate chemical shifts:



6. Propose structures for compounds that fit the following data:

- a. $C_5H_{10}O$ $\delta = 0.95$ ppm (6H, doublet)
 $\delta = 2.10$ ppm (3H, singlet)
 $\delta = 2.43$ ppm (1H, multiplet)



- b. $C_9H_{11}Br$ $\delta = 2.15$ ppm (2H, quintet)
 $\delta = 2.75$ ppm (2H, triplet)
 $\delta = 3.38$ ppm (2H, triplet)
 $\delta = 7.22$ ppm (5H, singlet)

