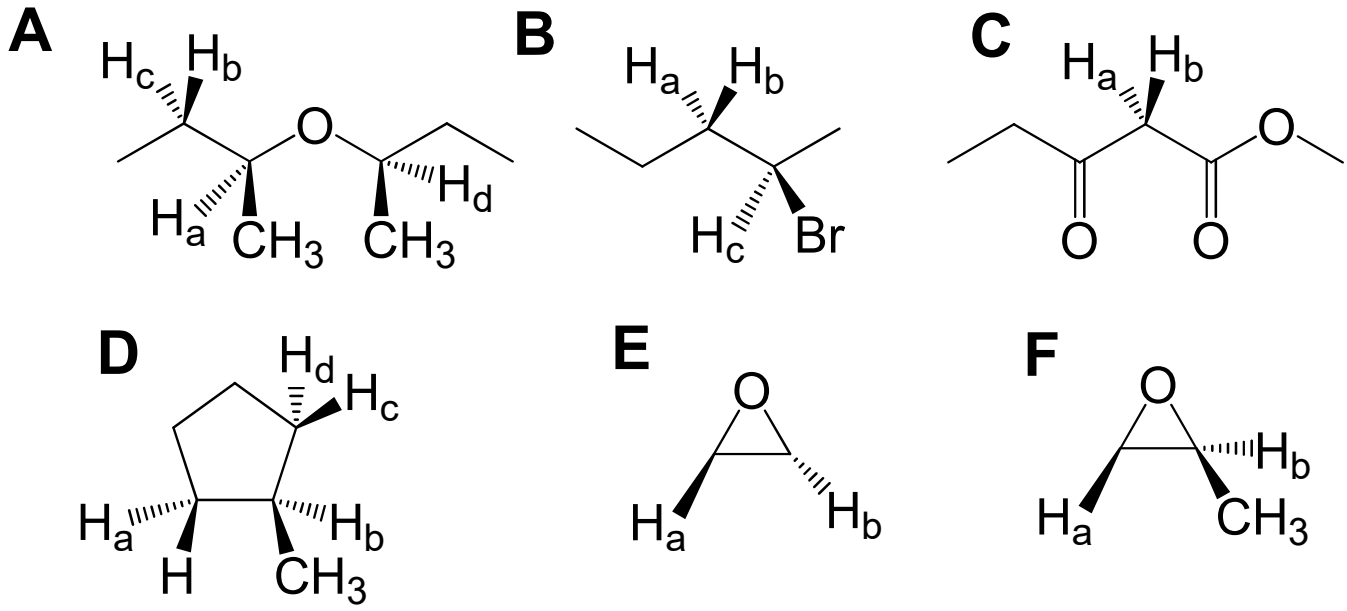
WORKSHEET II

1. On a 90 MHz spectrometer, calculate the frequency at which a proton absorbs if it appears at 4.20 ppm.

2. Using a 60 MHz spectrometer, the protons in dichloromethane appear at 5.30 ppm. When the same sample is placed in a 100 MHz instrument, where does the signal appear?
A) 8.33 B) 5.30 C) 3.18 D) cannot be determined from information given

3. State the relationship between the protons indicated in the structure below (as: equivalent, enantiotopic, diastereotopic, or unrelated)



4. The chair form of cyclohexane has protons in two distinct environments, axial and equatorial. When the proton NMR of cyclohexane is run on a 100-MHz instrument at 23°C, only one signal for the compound is observed. Explain this apparent contradiction.

5. How might the proton spectrum of ultrapure dimethylamine, $(CH_3)_2NH$, differ from the spectrum of this compound to which D_2O has been added?

6. Predict the number of signals expected (disregarding splitting) in the ^1H spectrum of the following compounds:

(a) *m*-xylene (1,3-dimethylbenzene)
(b) *o*-chlorophenol (2-chlorophenol)
(c) dibutyl ether
(d) 1,1-dimethylcyclobutane
(e) *m*-dichlorobenzene (1,3-dichlorobenzene)

7. Predict the number of signals expected, their splitting, and their relative area in the ^{1}H-NMR spectrum of the following compounds

(a) $CH_3CH_2OCH_3$
(b) $(CH_3)_3CCHO$
(c) 2-methylpropane (isobutane)
(d) 1,2-dichloroethane ($ClCH_2CH_2Cl$)

8. Deduce the identity of the following compound from the ^{1}H-NMR data given.

(a) $C_3H_3Cl_5$: δ 4.5 (1H, triplet), 6.1 (2H, doublet) (ppm)
(b) C_4H_7BrO: δ 2.2 (3H, singlet), 3.5 (2H, triplet), 4.5 (2H, triplet) (ppm)
(c) $C_3H_6Br_2$: δ 2.4 (2H, quintet), 3.5 (4H, triplet) (ppm)
(d) $C_5H_{10}O$: δ 1.1 (6H, doublet), 2.2 (3H, singlet), 2.5 (1H, septet) (ppm)
(e) $C_6H_8O_4$: δ 3.9 (6H, singlet), 6.1 (2H, singlet) (ppm)
(f) $C_7H_{12}O_4$: δ 1.3 (6H, triplet), 3.4 (2H, singlet), 4.2 (4H, quartet) (ppm)
(g) $C_5H_{12}O$: δ 1.0 (3H, triplet), 1.2-1.8 (6H, multiplet), 3.0 (1H, broad singlet), 3.8 (2H, triplet) (ppm)
(h) $C_7H_7NO_3$: δ 3.9 (3H, singlet), 6.9 (2H, doublet), 8.1 (2H, doublet) (ppm)
(i) $C_8H_{18}O$: δ 0.89 (6H, doublet), 1.87 (1H, multiplet), 3.17 (2H, doublet)(ppm)
(j) $C_6H_{10}O_2$: δ 2.19 (3H, singlet), 2.70 (2H, singlet) (ppm)
(k) $C_4H_{11}N$: δ 0.90 (3H, triplet), 1.07 (3H, doublet), 1.14 (2H, broad singlet), 1.34 (2H, multiplet), 2.79 (1H, multiplet) (ppm)

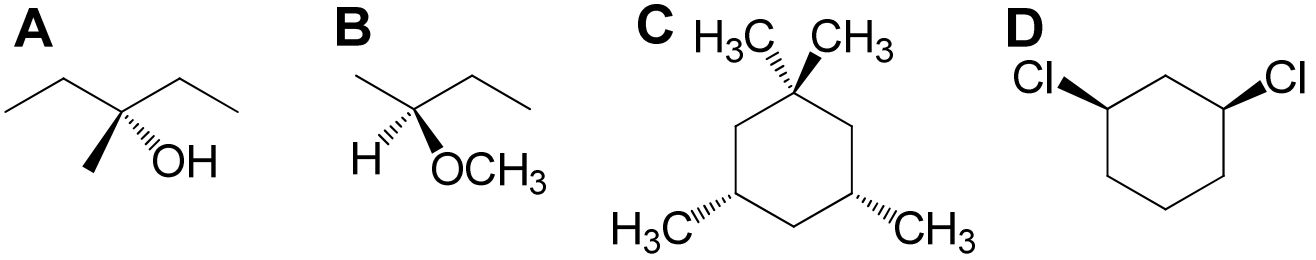
9. What is the approximate chemical shift of an alkynyl carbon in ^{13}C-NMR spectroscopy?

A) 10 ppm B) 30 ppm C) 70 ppm D) 120 ppm E) 200 ppm

10. Predict the number of signals expected in the proton spin decoupled ^{13}C-NMR spectrum of the following compounds:

(a) *o*-diethylbenzene (1,2-diethylbenzene).
(b) *p*-diethylbenzene (1,4-diethylbenzene).

11. Predict the number of signals expected (disregarding splitting) in the ^{1}H-NMR and in the proton spin decoupled ^{13}C NMR spectra of the compound shown below.



12. Deduce the identity of the following compound from the ^{13}C NMR data given.
C_9H_{12}: δ 21.3 (quartet), 127.2 (doublet), 138.0 (singlet) (ppm)

13. Deduce the identity of the following compound from the given spectral data.
(a) $C_7H_{10}O_2$: ^1H-NMR, δ 1.16 (3H, singlet), 2.21 (2H, singlet)
^{13}C-NMR: δ 216.25 (singlet), 52.57 (singlet), 34.51 (triplet), 20.22 (quartet) (ppm)

(b) C_3H_4BrN: ^1H-NMR, δ 2.98 (2H, triplet), 3.53 (2H, triplet)
^{13}C-NMR: δ 21.05 (triplet), 23.87 (triplet), 118.08 (singlet) (ppm); IR, 2963, 2254 cm^{-1}

(c) $C_5H_{10}O$: ^1H-NMR, δ 1.2 (6H, doublet), 2.1 (3H, singlet), 2.8 (1H, septet) (ppm)
IR: 2980, 1710 cm^{-1}; MS, *m/z* 71, 43

(d) C_8H_{10}: ^1H-NMR, δ 1.20 (3H, triplet), 2.60 (2H, quartet), 7.12 (5H, multiplet) (ppm)
IR: 3050, 2970, 1600 cm^{-1}; MS, *m/z* 91

(e) $C_4H_8O_2$: ^1H-NMR (δ) 1.23 (3H, triplet), 2.00 (3H, singlet), 4.02 (2H, quartet) (ppm)
IR: 2980, 1740 cm-1

(f) C_8H_{14} : IR (cm^{-1}): 2950, 2180; ^1H-NMR (δ): 0.9 (3H, t), 1.0 (9H, s), 2.3 (2H, q) (ppm).

(g) $C_4H_8O_3$: IR (cm^{-1}): 2800-3300 (broad), 2950, 1750; ^{13}C-NMR (δ): 17.7 (q), 65.4 (q), 72.3 (d), 210.8 (s) (ppm)

(h) C_6H_{10}: IR (cm^{-1}): 2950, 2230; ^1H-NMR (δ): 2.0 (1H, septet), 1.8 (3H, s), 0.9 (6H, d) ppm
^{13}C-NMR (δ): 78, 72, 45, 18, 15 ppm

(i) $C_5H_8Cl_2$: IR (cm^{-1}): 2950; ^1H-NMR (δ): 1.4 (4H, t), 1.2 (4H, t) ppm; ^{13}C-NMR (δ): 62, 26, 23 ppm

(j) $C_7H_{14}O_2$: IR (cm^{-1}): 2950, 1740; ^1H-NMR (δ): 0.9 (9H, s), 1.0 (3H, t), 2.3 (2H, q) ppm
^{13}C-NMR (δ): 185, 78, 29, 14, 12 ppm

(k) $C_5H_{10}O$: IR (cm^{-1}): 2950, 1720; ^1H-NMR (δ): 2.6 (1H, septet), 2.1 (3H, s), 1.0 (6H, d) ppm
^{13}C-NMR (δ): 195, 42, 18, 11 ppm

(l) C_9H_7Cl: IR (cm^{-1}): 3050, 2950, 2220, 1620; ^1H-NMR (d): 7.8 (2H, d), 7.2 (2H, d), 2.1 (3H, s) ppm
^{13}C-NMR: 140, 132, 125, 122, 88, 83, 18 ppm

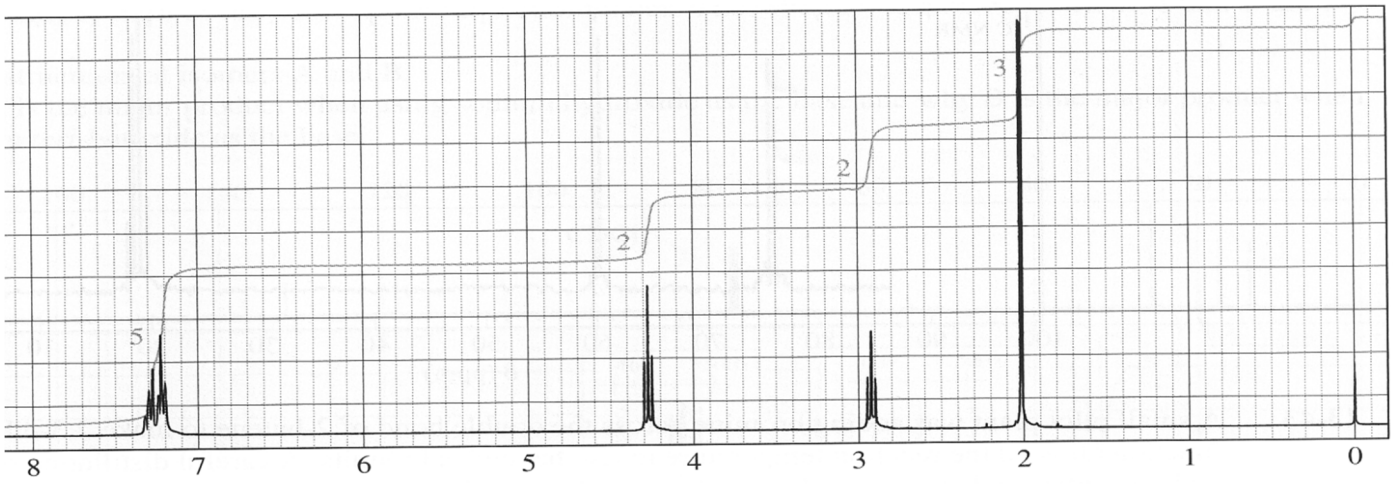
(m) $C_7H_{16}O$: IR (cm^{-1}): 3200-3600 (broad), 2950; ^1H-NMR (δ): 2.9 (1H, broad s), 1.2 (6H, q), 0.9 (9H, t) ppm; ^{13}C-NMR (δ): 70, 25, 12 ppm

(n) $C_5H_{10}O$: IR (cm^{-1}): 2950; ^1H-NMR (δ): 3.5 (4H, s), 0.9 (6H, s) ppm; ^{13}C-NMR (δ): 64, 41, 12 ppm

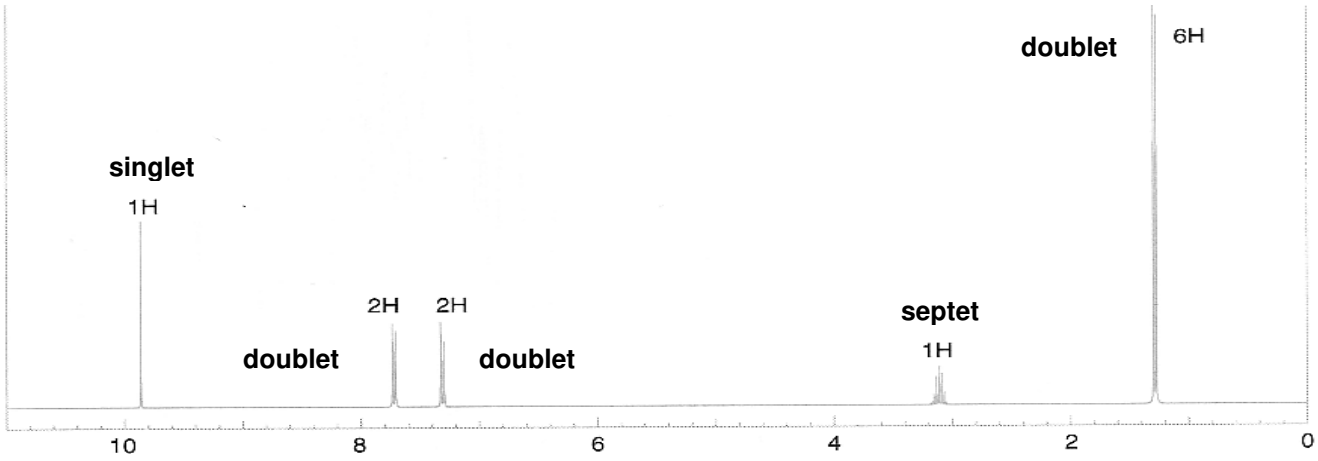
(o) $C_7H_{16}O$: IR (cm^{-1}): 3200-3600 (broad), 2950; ^1H-NMR (δ): 2.8 (1H, broad s), 1.0 (6H, s), 0.9 (9H, s) ppm; ^{13}C-NMR (δ): 68, 39, 16, 13 ppm

14. Deduce the identity of the following compound from the ^{1}H- NMR spectrum and the data given.

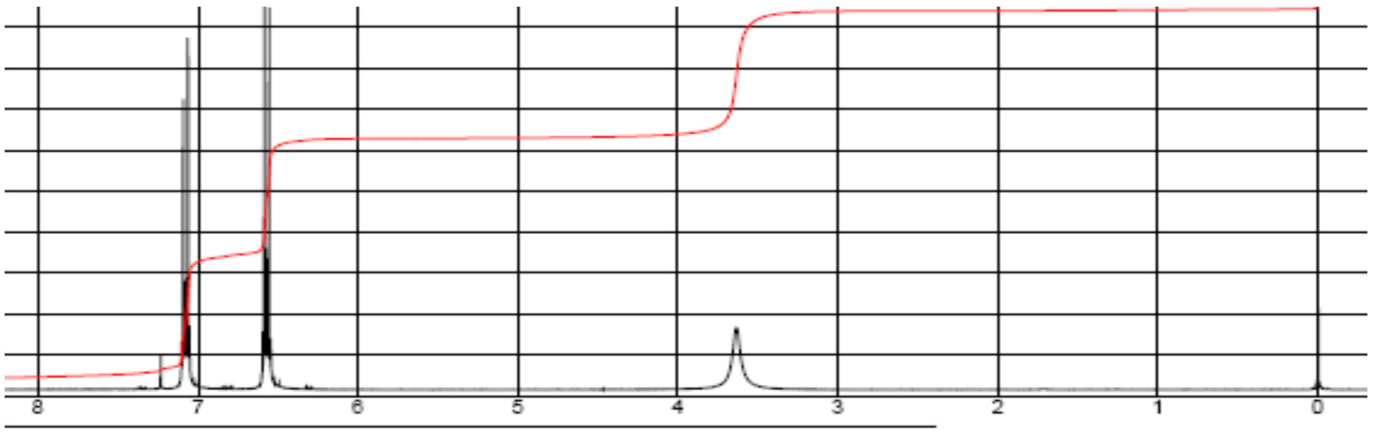
A $C_{10}H_{12}O_2$



B $C_{10}H_{12}O$

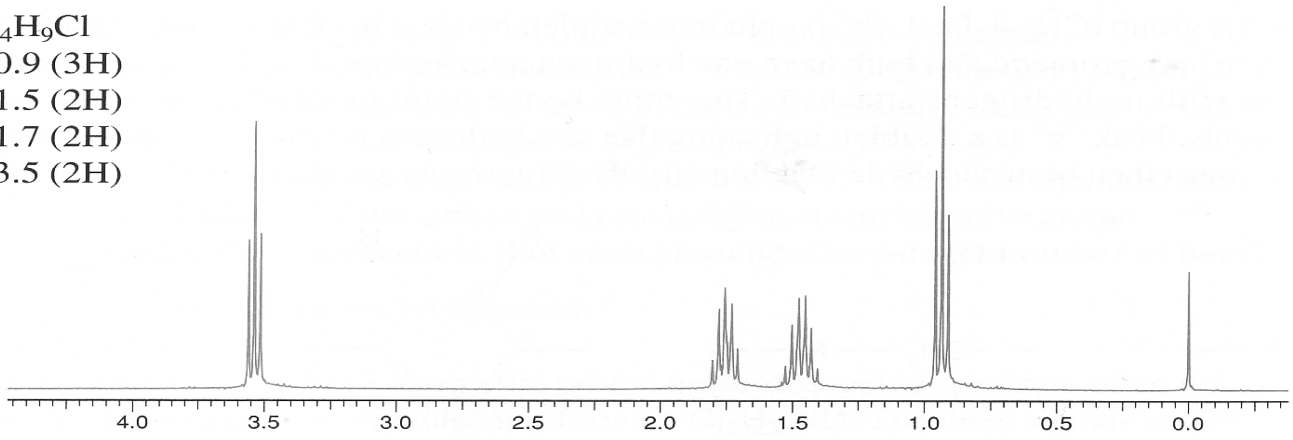


C C_6H_6NCl



D

C_4H_9Cl
δ0.9 (3H)
δ1.5 (2H)
δ1.7 (2H)
δ3.5 (2H)



E

$C_6H_{14}O$
δ0.9 (6H)
δ1.6 (4H)
δ3.4 (4H)