

**Organic Chemistry, 6e (Wade)**  
**Chapter 13: Nuclear Magnetic Resonance Spectroscopy**

4) How many nuclear spin states are allowed for the  $^1\text{H}$  nucleus?

- A) 1
- B) 2
- C) 3
- D) 4
- E) 10

Answer: B

Diff: 1

7) Electromagnetic radiation in the \_\_\_\_\_ region is used in  $^1\text{H}$  NMR spectroscopy.

- A) radio wave
- B) ultraviolet
- C) infrared
- D) microwave
- E) X-ray

Answer: A

Diff: 1

8) \_\_\_\_\_ is commonly used as an internal reference in NMR spectroscopy; its signal is assigned  $\delta = 0$  in  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopy.

Answer: Tetramethylsilane,  $(\text{CH}_3)_4\text{Si}$

Diff: 2

11) The protons marked  $\text{H}_a$  and  $\text{H}_b$  in the molecule below are \_\_\_\_\_.

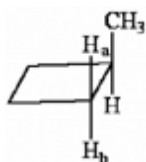


- A) chemically equivalent
- B) enantiotopic
- C) diastereotopic
- D) endotopic
- E) none of the above

Answer: A

Diff: 2

12) The protons marked  $\text{H}_a$  and  $\text{H}_b$  in the molecule below are \_\_\_\_\_.

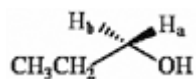


- A) chemically equivalent
- B) enantiotopic
- C) diastereotopic
- D) endotopic
- E) none of the above

Answer: C

Diff: 3

13) The protons marked  $H_a$  and  $H_b$  in the molecule below are \_\_\_\_\_.



- A) chemically equivalent
- B) enantiotopic
- C) diastereotopic
- D) endotopic
- E) none of the above

Answer: B

Diff: 3

15) 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?

Answer: N-H signal will broaden or disappear upon addition of  $D_2O$  as rapid hydrogen exchange occurs.

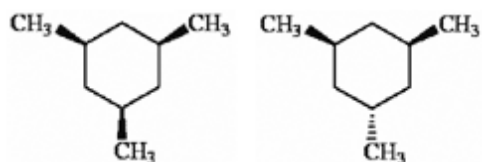
Diff: 2

16) Give one reason why  $^{13}C$  NMR is less sensitive than  $^1H$  NMR.

Answer: Natural isotopic abundance of  $^{13}C$  is about 100 times less than that of  $^1H$  or gyromagnetic ratio of  $^{13}C$  is much smaller.

Diff: 2

18) How might the two trimethylcyclohexane isomers shown below be most readily distinguished using NMR?



Answer: Number of signals in  $^{13}C$  NMR, 3 signals versus 6.

Diff: 3

19) What multiplicities are observed for the signals in the off-resonance decoupled  $^{13}\text{C}$  spectrum of 2-chloropropene?

- A) 3 singlets
- B) 2 singlets and a doublet
- C) a singlet and 2 doublets
- D) a singlet, a doublet and a triplet
- E) a singlet, a triplet, and a quartet

Answer: E

Diff: 1

20) What multiplicities are observed in the off-resonance decoupled  $^{13}\text{C}$  spectrum of 2,3-dimethyl-but-2-ene?

Answer: a singlet and a quartet

Diff: 2

21) Predict the number of signals expected (disregarding splitting) in the  $^1\text{H}$  spectrum of *m*-xylene (1,3-dimethylbenzene).

Answer: 4

Diff: 2

22) Predict the number of signals expected (disregarding splitting) in the  $^1\text{H}$  spectrum of *o*-chlorophenol (2-chlorophenol).

Answer: 5

Diff: 2

23) Predict the number of signals expected (disregarding splitting) in the  $^1\text{H}$  spectrum of dibutyl ether.

Answer: 4

Diff: 2

24) Predict the number of signals expected (disregarding splitting) in the  $^1\text{H}$  spectrum of 1,1-dimethylcyclobutane.

Answer: 3

Diff: 2

25) Predict the number of signals expected in the proton spin decoupled  $^{13}\text{C}$  spectrum of *cis*-1,3-dimethylcyclopentane.

Answer: 4

Diff: 3

28) Predict the number of signals expected in the proton spin decoupled  $^{13}\text{C}$  spectrum of *m*-dichlorobenzene (1,3-dichlorobenzene).

Answer: 4

Diff: 2

29) Predict the number of signals expected in the proton spin decoupled  $^{13}\text{C}$  spectrum of *p*-dibromobenzene (1,4-dibromobenzene).

Answer: 2

Diff: 2

31) Predict the number of signals expected, their splitting, and their relative area in the  $^1\text{H}$  NMR spectrum of  $\text{CH}_3\text{CH}_2\text{OCH}_3$ .

Answer: 3 signals: (3H, triplet); (2H, quartet); (3H, singlet)

Diff: 1

32) Predict the number of signals expected, their splitting, and their relative area in the  $^1\text{H}$  NMR spectrum of  $(\text{CH}_3)_3\text{CCHO}$ .

Answer: 2 signals: (9H, singlet); (1H, singlet)

Diff: 2

33) Predict the number of signals expected, their splitting, and their relative area in the  $^1\text{H}$  NMR spectrum of 2-methylpropane (isobutane).

Answer: 2 signals: (9H, doublet); (1H, 10 line pattern)

Diff: 2

34) Predict the number of signals expected, their splitting, and their relative area in the  $^1\text{H}$  NMR spectrum of 1,2-dichloroethane ( $\text{ClCH}_2\text{CH}_2\text{Cl}$ ).

Answer: 1 signal: singlet

Diff: 3

35) Deduce the identity of the following compound from the  $^1\text{H}$  NMR data given.

$\text{C}_8\text{H}_{10}\text{O}$ :  $\delta$  3.4 (3H, singlet), 4.5 (2H, singlet), 7.2 (5H, singlet) (ppm)

Answer:  $\text{PhCH}_2\text{OCH}_3$

Diff: 1

36) Deduce the identity of the following compound from the  $^1\text{H}$  NMR data given.

$\text{C}_9\text{H}_{10}\text{O}_2$ :  $\delta$  2.2 (3H, singlet), 5.0 (2H, singlet), 7.2 (5H, singlet) (ppm)

Answer:  $\text{PhCH}_2\text{O}_2\text{CCH}_3$

Diff: 2

37) Deduce the identity of the following compound from the  $^1\text{H}$  NMR data given.

$\text{C}_3\text{H}_3\text{Cl}_5$ :  $\delta$  4.5 (1H, triplet), 6.1 (2H, doublet) (ppm)

Answer:  $\text{Cl}_2\text{CHCHClCHCl}_2$

Diff: 2

38) Deduce the identity of the following compound from the  $^1\text{H}$  NMR data given.

$\text{C}_4\text{H}_7\text{BrO}$ :  $\delta$  2.2 (3H, singlet), 3.5 (2H, triplet), 4.5 (2H, triplet) (ppm)

Answer:  $\text{CH}_3\text{COCH}_2\text{CH}_2\text{Br}$

Diff: 2

39) Deduce the identity of the following compound from the  $^1\text{H}$  NMR data given.

$\text{C}_3\text{H}_6\text{Br}_2$ :  $\delta$  2.4 (2H, quintet), 3.5 (4H, triplet) (ppm)

Answer:  $\text{BrCH}_2\text{CH}_2\text{CH}_2\text{Br}$

Diff: 1

40) Deduce the identity of the following compound from the  $^1\text{H}$  NMR data given.

$\text{C}_5\text{H}_{10}\text{O}$ :  $\delta$  1.1 (6H, doublet), 2.2 (3H, singlet), 2.5 (1H, septet) (ppm)

Answer:  $\text{CH}_3\text{COCH}(\text{CH}_3)_2$

Diff: 2

44) Deduce the identity of the following compound from the  $^1\text{H}$  NMR data given.

$\text{C}_7\text{H}_7\text{NO}_3$ :  $\delta$  3.9 (3H, singlet), 6.9 (2H, doublet), 8.1 (2H, doublet) (ppm)

Answer: *p*-nitroanisole ( $p\text{-O}_2\text{NC}_6\text{H}_4\text{OCH}_3$ )

Diff: 3

45) Deduce the identity of the following compound from the  $^1\text{H}$  NMR data given.

$\text{C}_8\text{H}_{18}\text{O}$ :  $\delta$  0.89 (6H, doublet), 1.87 (1H, multiplet), 3.17 (2H, doublet)(ppm)

Answer:  $[(\text{CH}_3)_2\text{CHCH}_2]_2\text{O}$

Diff: 2

46) Deduce the identity of the following compound from the  $^1\text{H}$  NMR data given.

$\text{C}_6\text{H}_{10}\text{O}_2$ :  $\delta$  2.19 (3H, singlet), 2.70 (2H, singlet) (ppm)

Answer:  $\text{CH}_3\text{COCH}_2\text{CH}_2\text{COCH}_3$

Diff: 2

51) Deduce the identity of the following compound from the  $^{13}\text{C}$  NMR data given.

$\text{C}_4\text{H}_{10}\text{O}$ :  $\delta$  10.0 (quartet), 22.9 (quartet), 32.0 (triplet), 69.6 (doublet) (ppm)

Answer: butan-2-ol

Diff: 2

52) Deduce the identity of the following compound from the  $^{13}\text{C}$  NMR data given.

$\text{C}_8\text{H}_8\text{O}$ :  $\delta$  26.4 (quartet), 128.0 (doublet), 128.3 (doublet), 133.0 (doublet), 137.0 (singlet), 198.0 (singlet) (ppm)

Answer: acetophenone ( $\text{PhCOCH}_3$ )

Diff: 2

54) Deduce the identity of the following compound from the  $^1\text{H}$  NMR data given.

$\text{C}_4\text{H}_{11}\text{N}$ :  $\delta$  0.90 (3H, triplet), 1.07 (3H, doublet), 1.14 (2H, broad singlet), 1.34 (2H, multiplet), 2.79 (1H, multiplet) (ppm)

Answer: *sec*-butylamine

Diff: 2

55) Deduce the identity of the following compound from the  $^{13}\text{C}$  NMR data given.

$\text{C}_6\text{H}_{12}\text{O}$ :  $\delta$  29.80 (quartet), 30.82 (singlet), 56.53 (triplet), 203.36 (doublet) (ppm)

Answer:  $(\text{CH}_3)_3\text{CCH}_2\text{CHO}$

Diff: 2

56) Deduce the identity of the following compound from the  $^{13}\text{C}$  NMR data given.

$\text{C}_4\text{H}_8\text{O}$ :  $\delta$  11.97 (triplet), 33.54 (triplet), 67.03 (doublet) (ppm)

Answer: cyclobutanol

Diff: 2

57) Deduce the identity of the following compound from the spectral data given.

$\text{C}_9\text{H}_{10}\text{O}_2$ :  $^{13}\text{C}$  NMR,  $\delta$  18.06 (quartet), 45.40 (doublet), 127.32 (doublet), 127.55 (doublet), 128.61 (doublet), 139.70 (singlet) (ppm), 180.98 (singlet); IR, broad 3500-2800, 1708  $\text{cm}^{-1}$

Answer:  $\text{PhCH}(\text{CH}_3)\text{CO}_2\text{H}$

Diff: 3

58) Deduce the identity of the following compound from the spectral data given.

$\text{C}_5\text{H}_{10}\text{O}$ :  $^1\text{H}$  NMR,  $\delta$  1.2 (6H, doublet), 2.1 (3H, singlet), 2.8 (1H, septet) (ppm); IR, 2980, 1710  $\text{cm}^{-1}$ ; MS,  $m/z$  71, 43

Answer:  $(\text{CH}_3)_2\text{CHCOCH}_3$

Diff: 3

59) Deduce the identity of the following compound from the spectral data given.

$C_8H_{10}$ :  $^1H$  NMR,  $\delta$  1.20 (3H, triplet), 2.60 (2H, quartet), 7.12 (5H, singlet) (ppm); IR, 3050, 2970, 1600  $cm^{-1}$ ; MS,  $m/z$  91  
Answer:  $PhCH_2CH_3$

Diff: 2

60) Deduce the identity of the following compound from the spectral data given.

$C_4H_8O_2$ :  $^1H$  NMR,  $\delta$  1.23 (3H, triplet), 2.00 (3H, singlet), 4.02 (2H, quartet) (ppm); IR, 2980, 1740  $cm^{-1}$   
Answer:  $CH_3CO_2CH_2CH_3$

Diff: 3

62) The  $^1\text{H}$  NMR spectrum of ethanol is acquired and the hydroxyl signal appears as a singlet instead of a triplet. Offer an explanation.

Answer: A fast exchange of the hydroxyl H from one ethanol molecule to another is occurring. This rapidly exchanging H produces a single, unsplit absorption at an average field.

Diff: 3

63) You have a sample and its  $^1\text{H}$  NMR spectrum. You know your sample contains O atoms but not N atoms, and you suspect that your sample may be an alcohol. What common spectroscopic technique might you use to confirm your suspicion?

Answer: Take an IR spectrum and look for the O–H stretch or add some  $\text{D}_2\text{O}$  to the sample and reacquire the  $^1\text{H}$  NMR to see if a peak broadens or disappears.

Diff: 2

64) If a molecule contains 4 elements of unsaturation and signals in the  $^1\text{H}$  NMR spectrum between  $\delta$  7.0 and 8.0 ppm, what structural group is likely to be present?

A) a carbonyl group

B) an aromatic ring

C) a hydroxyl group

D) a cyclohexyl ring

E) a carbon-carbon triple bond

Answer: B

Diff: 1

67) Deduce the identity of the compound whose molecular formula is  $\text{C}_4\text{H}_8\text{O}_3$  from the spectral data provided: IR ( $\text{cm}^{-1}$ ): 2800-3300 (broad), 2950, 1750;  $^{13}\text{C}$  NMR ( $\delta$ ): 17.7 (q), 65.4 (q), 72.3 (d), 210.8 (s) (ppm)

Answer:  $\text{CH}_3\text{OCH}(\text{CH}_3)\text{CO}_2\text{H}$

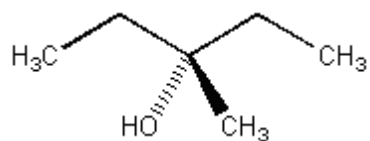
Diff: 2

68) Why is carbon-hydrogen splitting not a major part of  $^1\text{H}$  NMR spectra?

Answer: Most of the carbons are  $^{12}\text{C}$  which does not exhibit coupling to  $^1\text{H}$ .

Diff: 2

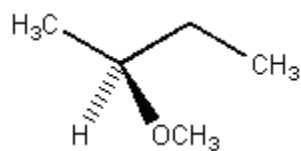
71) Predict the number of signals expected (disregarding splitting) in the  $^1\text{H}$  NMR spectrum of the compound shown below.



Answer: 4

Diff: 2

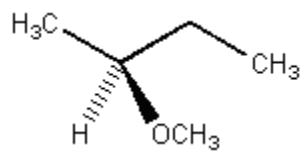
74) Predict the number of signals expected (disregarding splitting) in the  $^1\text{H}$  NMR spectrum of the compound shown below.



Answer: 5

Diff: 2

75) Predict the number of signals expected in the proton spin decoupled  $^{13}\text{C}$  NMR spectrum of the compound shown below.



Answer: 5

Diff: 2

81) Provide a structure that is consistent with the data below.

$C_6H_{10}$

IR ( $cm^{-1}$ ): 2950, 2230

$^1H$  NMR (d): 2.0 (1H, septet), 1.8 (3H, s), 0.9 (6H, d)

$^{13}C$  NMR (d): 78 (s), 72 (s), 45 (d), 18 (q), 15 (q)

Answer:  $(CH_3)_2CHC\equiv CCH_3$

Diff: 2

82) Provide a structure that is consistent with the data below.

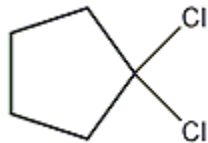
$C_5H_8Cl_2$

IR ( $cm^{-1}$ ): 2950

$^1H$  NMR (d): 1.4 (4H, t), 1.2 (4H, t)

$^{13}C$  NMR (d): 62 (s), 26 (t), 23 (t)

Answer:



Diff: 3

83) Provide a structure that is consistent with the data below.

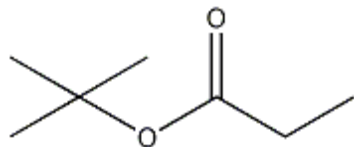
$C_7H_{14}O_2$

IR ( $cm^{-1}$ ): 2950, 1740

$^1H$  NMR (d): 2.3 (2H, q), 1.0 (3H, t), 0.9 (9H, s)

$^{13}C$  NMR (d): 185 (s), 78 (s), 29 (t), 14 (q), 12 (q)

Answer:



Diff: 3

85) Provide a structure that is consistent with the data below.

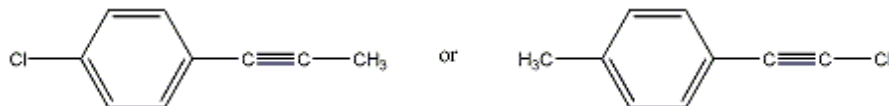
$C_9H_7Cl$

IR ( $cm^{-1}$ ): 3050, 2950, 2220, 1620

$^1H$  NMR (d): 7.8 (2H, d), 7.2 (2H, d), 2.1 (3H, s)

$^{13}C$  NMR (d): 140 (s), 132, (s), 125 (d), 122 (d), 88 (s), 83 (s), 18 (q)

Answer:



Diff: 3

86) Provide a structure that is consistent with the data below.

$C_7H_{16}O$

IR ( $cm^{-1}$ ): 3200-3600 (broad), 2950

$^1H$  NMR (d): 2.9 (1H, broad s), 1.2 (6H, q), 0.9 (9H, t)

$^{13}C$  NMR (d): 70 (s), 25 (t), 12 (q)

Answer:  $(CH_3CH_2)_3COH$

Diff: 3

87) Provide a structure that is consistent with the data below.

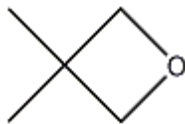
$C_5H_{10}O$

IR ( $cm^{-1}$ ): 2950

$^1H$  NMR (d): 3.5 (4H, s), 0.9 (6H, s)

$^{13}C$  NMR (d): 64 (t), 41 (s), 12 (q)

Answer:



Diff: 3

88) Provide a structure that is consistent with the data below.

$C_7H_{16}O$

IR ( $cm^{-1}$ ): 3200-3600 (broad), 2950

$^1H$  NMR (d): 2.8 (1H, broad s), 1.0 (6H, s), 0.9 (9H, s)

$^{13}C$  NMR (d): 68 (s), 39 (s), 16 (q), 13 (q)

Answer:  $(CH_3)_3CC(CH_3)_2OH$

Diff: 3

90) Provide a structure that is consistent with the data below.

$C_4H_8O$

IR ( $cm^{-1}$ ): 2950

$^1H$  NMR (d): 3.2 (4H, t), 1.2 (4H, t)

$^{13}C$  NMR (d): 68 (t), 27 (t)

Answer:



Diff: 3

91) In the  $^1\text{H}$  NMR spectrum of bromoethane the methylene group is split into a quartet by the  $\alpha$  and  $\beta$  nuclear spins of the protons on the neighboring methyl group. If the external magnetic field,  $B^\circ$ , directs upward, which sequence of nuclear spins contributes to the second farthest peak down field within the spin-spin splitting pattern?

- A)  $\uparrow\downarrow\downarrow$
- B)  $\uparrow\downarrow\uparrow$
- C)  $\uparrow\uparrow\uparrow$
- D)  $\downarrow\downarrow\downarrow$
- E)  $\uparrow\uparrow\downarrow\downarrow$

Answer: B

Diff: 3

99) Compound **I** has a molecular formula of  $C_7H_{16}$ . In  $^{13}C$  NMR, compound **I** gave 3 peaks and in  $^1H$  NMR it also gave 3 peaks, a doublet, a triplet and a multiplet. Provide a structure for compound **I**.

Answer:



Diff: 2