

1) Which compound would be expected to show intense IR absorption at  $3300\text{ cm}^{-1}$ ?

- A)  $\text{CH}_3\text{C}\equiv\text{CCH}_3$
- B) butane
- C) but-1-ene
- D)  $\text{CH}_3\text{CH}_2\text{C}\equiv\text{CH}$

Answer: D

2) Which compound would be expected to show intense IR absorption at  $2820$ ,  $2710$  and  $1705\text{ cm}^{-1}$ ?

- A)  $\text{CH}_3\text{COCH}_2\text{CH}_3$
- B)  $\text{PhCOCH}_3$
- C)  $\text{PhCHO}$
- D)  $\text{CH}_2=\text{CHCOCH}_3$

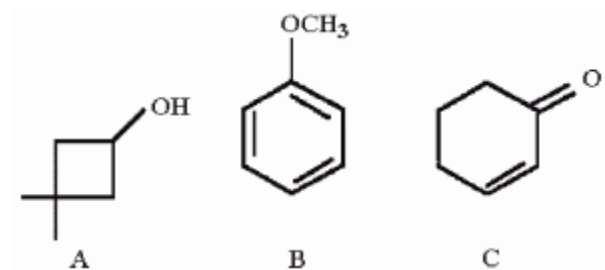
Answer: C

3) Which compound would be expected to show intense IR absorption at  $2250\text{ cm}^{-1}$ ?

- A)  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CO}_2\text{H}$
- B)  $(\text{CH}_3)_2\text{CHCH}_2\text{OH}$
- C)  $(\text{CH}_3)_2\text{CHCN}$
- D)  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CONH}_2$

Answer: C

4) Which compound would be expected to show intense IR absorption at  $1680\text{ cm}^{-1}$ ?



Answer: Compound C

5) Deduce a possible structure for the compound with the IR absorptions below.

$\text{C}_3\text{H}_3\text{Br}$ :  $3300$ ,  $2900$ ,  $2100\text{ cm}^{-1}$

Answer:  $\text{HC}\equiv\text{CCH}_2\text{Br}$

6) Deduce a possible structure for the compound with the IR absorptions below.

$\text{C}_3\text{H}_5\text{N}$ :  $2950$ ,  $2250\text{ cm}^{-1}$

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

7) Deduce a possible structure for the compound with the IR absorptions below.

$C_5H_8O$ : 2950, 1750  $cm^{-1}$

Answer: cyclopentanone

8) Deduce a possible structure for the compound with the IR absorptions below.

$C_4H_8O$ : 2950, 2820, 2715, 1715  $cm^{-1}$

Answer:  $CH_3CH_2CH_2CHO$

9) Deduce a possible structure for the compound with the IR absorptions below.

$C_6H_{10}$ : 3040, 2980, 1660  $cm^{-1}$

Answer: cyclohexene

10) How could IR spectroscopy be used to distinguish between the following pair of compounds?

$CH_3OCH_2CH_3$  and  $CH_3CH_2CH_2OH$

Answer: O-H stretch at 3300  $cm^{-1}$

11) How could IR spectroscopy be used to distinguish between the following pair of compounds?

$HOCH_2CH_2CHO$  and  $CH_3CH_2CO_2H$

Answer: A carboxylic acid will have a very broad O-H absorption near 3000  $cm^{-1}$ ; an aldehyde has characteristic C-H stretches at 2820 and 2720  $cm^{-1}$ .

12) How could IR spectroscopy be used to distinguish between the following pair of compounds?

$CH_3COCH=CHCH_2CH_3$  and  $CH_3COCH_2CH_2CH=CH_2$

Answer: C=O absorption in conjugated carbonyl appears at lower wavenumber

13) How could IR spectroscopy be used to distinguish between the following pair of compounds?

$CH_3CH_2C\equiv CH$  and  $CH_3C\equiv CCH_3$

Answer: Terminal alkyne stretch at 3300  $cm^{-1}$ , lower intensity C=C absorption in internal alkyne

14) Ethyne ( $HC\equiv CH$ ) does not show IR absorption in the region 2000-2500  $cm^{-1}$  because:

A) C-H stretches occur at lower energies.

B) C=C stretches occur at about 1640  $cm^{-1}$ .

C) there is no change in the dipole moment when the C=C bond in ethyne stretches.

D) there is a change in the dipole moment when the C=C bond in ethyne stretches.

Answer: C

15) Describe the molecular ion region in the mass spectrum of  $\text{CH}_3\text{CH}_2\text{Br}$ .

Answer: The natural abundance of the isotopes  $^{79}\text{Br}$  and  $^{81}\text{Br}$  are about the same; therefore, there will be peaks of equal intensity at  $m/z$  108 and 110.

16) 2-Methylhexane shows an intense peak in the mass spectrum at  $m/z = 43$ . Propose a likely structure for this fragment.

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

17) Which compound would show a larger than usual M+2 peak in the mass spectrum?

- A)  $\text{CH}_3\text{CH}_2\text{SCH}_3$
- B)  $(\text{CH}_3)_2\text{CHNH}_2$
- C)  $\text{CH}_3\text{CH}_2\text{CO}_2\text{H}$
- D)  $\text{CH}_3(\text{CH}_2)_2\text{CH}_3$

Answer: A

18) Which compound would be expected to show intense IR absorption at  $1715\text{ cm}^{-1}$ ?

- A)  $(\text{CH}_3)_2\text{CHNH}_2$
- B) hex-1-yne
- C) 2-methylhexane
- D)  $(\text{CH}_3)_2\text{CHCO}_2\text{H}$

Answer: D

19) Which compound would be expected to show intense IR absorption at  $3363, 3185, 1660\text{ cm}^{-1}$ ?

- A)  $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$
- B)  $(\text{CH}_3)_2\text{CHNH}_2$
- C)  $\text{CH}_3\text{CH}_2\text{CONH}_2$
- D) but-1-ene

Answer: C

20) Which compound would be expected to show intense IR absorption at  $1746\text{ cm}^{-1}$ ?

- A)  $\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3$
- B)  $\text{CH}_3\text{CH}_2\text{CN}$
- C)  $\text{CH}_3\text{CO}_2\text{CH}_2\text{CH}_3$
- D)  $\text{CH}_3\text{CH}_2\text{SCH}_3$

Answer: C

21) Absorption \_\_\_\_\_ is the measurement of the amount of light absorbed by a compound as a function of the wavelength of light.

Answer: spectroscopy

22) An infrared wavelength of  $4.48\mu\text{m}$  is equivalent to a wavenumber of \_\_\_\_\_  $\text{cm}^{-1}$ .

Answer: 2230

23) An infrared wavelength of  $5.81\mu\text{m}$  is equivalent to a wavenumber of \_\_\_\_\_  $\text{cm}^{-1}$ .

Answer: 1720

24) Which has the higher speed in a vacuum, ultraviolet or infrared light?

Answer: They have the same speed.

2

25) The wavelength and frequency of a given wave of electromagnetic radiation are \_\_\_\_\_ proportional.

Answer: inversely

2

26) The energy of a photon is \_\_\_\_\_ proportional to its wavelength.

Answer: inversely

1

27) The energy of a photon is \_\_\_\_\_ proportional to its frequency.

Answer: directly

1

28) In what units are frequency values typically given?

Answer: Hertz or cycles/sec or  $\text{sec}^{-1}$

1

29) In an IR spectrometer, the \_\_\_\_\_ uses prisms or diffraction gratings to allow only one frequency of light to enter the detector at a time.

Answer: monochromator

2

30) Which region of the electromagnetic spectrum, IR or UV, contains photons of the higher energy?

Answer: UV

2

31) Which region of the electromagnetic spectrum, radio or visible, is characterized by waves of shorter wavelength?

Answer: visible

2

32) Which region of the electromagnetic spectrum, IR or X-ray, is characterized by waves of lower frequency?

Answer: IR

2

33) Which has a lower characteristic stretching frequency, the C–H or C–D bond? Explain briefly.

Answer: C–D; heavier atoms vibrate more slowly

3

34) Which has a lower characteristic stretching frequency, the C=O bond or the C–O bond? Explain briefly.

Answer: Stronger bonds are generally stiffer, thus requiring more force to stretch or compress them. The C–O bond is the weaker of the two and hence has the lower stretching frequency.

3

35) The region of the IR spectrum which contains the most complex vibrations ( $600\text{-}1400\text{ cm}^{-1}$ ) is called the \_\_\_\_\_ region of the spectrum.

Answer: fingerprint

2

36) In order for a vibration mode to be observable in the IR, the vibration must change the \_\_\_\_\_ of the molecule.

Answer: dipole moment

2

37) What effect does conjugation typically have on the frequency at which absorption by  $\text{C}=\text{C}$  occurs?

A) Conjugation decreases the frequency at which absorption occurs.

B) Conjugation increases the frequency at which absorption occurs.

C) Conjugation does not affect the frequency at which absorption occurs.

Answer: A

2

38) Describe the fate of a molecule from introduction to detection in a mass spectrometer.

Answer: Upon introduction, sample molecules are ionized by an electron beam passing through a vacuum chamber. The resulting radical cation and fragment cations are accelerated into the flight tube of the magnet by a negatively charged plate. In the flight tube, the path of the ions is bent by the existing magnetic field. For a given magnetic field strength, only one  $m/z$  will be bent in such a way that its path matches the curvature of the tube and reaches the detector. The entire  $m/z$  range is scanned by varying the strength of the magnetic field.

2

39) When a high energy electron impacts molecule M in the ionization chamber, what type of species is initially produced?

A) cation

B) anion

C) radical

D) radical cation

E) radical anion

Answer: D

2

40) In a mass spectrum, the peak of greatest abundance is referred to as the \_\_\_\_\_.

Answer: base peak

1

41) What spectroscopic technique can be used to determine the molecular formula of a compound?

Answer: high resolution mass spectrometry

2

42) The natural abundances of chlorine's two major isotopes are  $^{35}\text{Cl}$  (75.5%) and  $^{37}\text{Cl}$  (24.5%). If the mass spectrum of chlorobenzene contains a peak at  $m/z$  114 with an abundance of 15.0%, calculate the % abundance of the peak at  $m/z$  112.

Answer: 46.2%

2

43) An \_\_\_\_\_ molecular ion peak usually indicates the presence of an odd number of nitrogen atoms in the molecule.

- A) even
- B) odd
- C) intense
- D) absent

Answer: B

1

44) The mass spectrum of alcohols often fail to exhibit detectable M peaks but instead show relatively large \_\_\_\_\_ peaks.

- A) M+1
- B) M+2
- C) M-16
- D) M-17
- E) M-18

Answer: E

2

45) How could IR spectroscopy be used to distinguish between the following pair of compounds?

$\text{CH}_2=\text{CHCH}_2\text{CH}(\text{CH}_3)_2$  and  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2$

Answer: C=C stretch around  $1640\text{ cm}^{-1}$ ; vinylic C-H stretch above  $3000\text{ cm}^{-1}$

1

46) How could IR spectroscopy be used to distinguish between the following pair of compounds?

$(\text{CH}_3)_3\text{N}$  and  $\text{CH}_3\text{NHCH}_2\text{CH}_3$

Answer: N-H absorption near  $3300\text{ cm}^{-1}$

2

47) Sodium borohydride can be used to reduce cyclohexanone to cyclohexanol. How could one use IR to determine if all starting material had been consumed?

Answer: Presence of C=O stretch would indicate incomplete reaction.

2

48) Which compound would be expected to show intense IR absorption at  $3367, 3282\text{ cm}^{-1}$ ?

- A) but-1-ene
- B)  $\text{PhCO}_2\text{H}$
- C)  $\text{CH}_3\text{OCH}_2\text{CH}_3$
- D)  $\text{PhCH}_2\text{NH}_2$

Answer: D

1

49) Which compound would be expected to show intense IR absorption at  $1640\text{ cm}^{-1}$ ?

- A) hex-1-ene
- B) 2-methylheptane
- C)  $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$
- D)  $\text{CH}_3\text{CH}_2\text{COCH}_3$

Answer: A

1

50) The two most abundant isotopes of boron are  $^{10}\text{B}$  and  $^{11}\text{B}$ , with  $^{11}\text{B}$  being about 4 times more abundant. In the mass spectrum of trimethylborate  $[(\text{CH}_3\text{O})_3\text{B}]$ , \_\_\_\_\_:

- A) the peaks at  $m/z$  103 and  $m/z$  104 have equivalent intensities
- B) the peak at  $m/z$  103 has an intensity which is 4 times that of the  $m/z$  104 peak
- C) the peak at  $m/z$  103 has an intensity which is 1/4 the intensity of the peak at  $m/z$  104
- D) none of the above

Answer: C

2

51) Absorption of what type of electromagnetic radiation results in ionization?

- A) X-rays
- B) radio waves
- C) microwaves
- D) ultraviolet light
- E) infrared light

Answer: A

2

52) Absorption of what type of electromagnetic radiation results in electronic transitions?

- A) X-rays
- B) radio waves
- C) microwaves
- D) ultraviolet light
- E) infrared light

Answer: D

2

53) Absorption of what type of electromagnetic radiation results in transitions among allowed rotational motions?

- A) X-rays
- B) radio waves
- C) microwaves
- D) ultraviolet light
- E) infrared light

Answer: C

2

54) Absorption of what type of electromagnetic radiation results in transitions among allowed vibrational motions?

- A) X-rays
- B) radio waves
- C) microwaves
- D) ultraviolet light
- E) infrared light

Answer: E

2

55) Absorption of what type of electromagnetic radiation results in transitions among allowed nuclear magnetic spin states?

- A) X-rays
- B) radio waves
- C) microwaves
- D) ultraviolet light
- E) infrared light

Answer: B

2

56) At approximately what wavenumber does one expect to find the carbon-carbon triple bond stretch in the IR spectrum of an alkyne?

Answer: 2100 - 2200  $\text{cm}^{-1}$

2

57) Which of the following fragment peaks would not be present in the mass spectrum of *n*-hexane?

- A) 87
- B) 71
- C) 57
- D) 43
- E) 29

Answer: A

1

58) A compound ( $\text{C}_5\text{H}_8\text{O}$ ) shows IR absorptions at 3600 and 3300  $\text{cm}^{-1}$ . Its  $^1\text{H}$  NMR spectrum contained singlets at  $\delta$  1.5, 2.2, and 2.9 (broad) (ppm) in a ratio of 6:1:1. Name this compound.

Answer: 2-methylbut-3-yn-2-ol

1

59) Provide an equation which relates the energy of a photon to its wavelength.

Answer:  $E = (hc)/\lambda$

1

60) The frequency of the stretching vibration of a bond in IR spectroscopy depends on what two quantities?

- A) the stiffness of the bond and the electronegativity of the atoms
- B) the electronegativity of the atoms and the nuclear charges of the atoms
- C) the masses of the atoms and the stiffness of the bond
- D) the nuclear charges of the atoms and the atomic radii
- E) the electronegativity of the atoms and the masses of the atoms

Answer: C

2

61) In IR spectroscopy, the C–O bond has a \_\_\_\_\_ frequency than the C–N bond because \_\_\_\_\_.

- A) higher, an O atom has more mass than an N atom
- B) lower, an O atom has more mass than an N atom
- C) higher, an O atom has more electronegativity than an N atom
- D) lower, an O atom has more electronegativity than an N atom
- E) higher, an O atom has an even number of neutrons

Answer: B

2

62) A nonlinear molecule with n atoms generally has \_\_\_\_\_ fundamental vibrational modes.

- A) 2n
- B) 2n - 2
- C) 3n
- D) 3n - 3
- E) 3n - 6

Answer: E

3

63) The IR spectrum of a sample contains absorptions at 3050, 2950, and 1620  $\text{cm}^{-1}$ . To what class of organic compound does this sample most likely belong?

- A) alkane
- B) alkene
- C) alkyne
- D) ester
- E) alcohol

Answer: B

2

64) How does the O–H stretch in the IR spectrum of a carboxylic acid differ from the O–H stretch of an alcohol?

Answer: Because of the unusually strong hydrogen bonding in carboxylic acids, the broad O–H stretch is shifted to about 3000  $\text{cm}^{-1}$  centered on top of the usual C–H absorption. This broad O–H absorption gives a characteristic overinflated shape to the peaks in the C–H region.

2

65) When a compound contains a sulfur atom, its mass spectrum contains a larger than usual \_\_\_\_\_ peak.

- A) M-2
- B) M-1
- C) M
- D) M+1
- E) M+2

Answer: E

3

66) Arrange the following regions of the electromagnetic spectrum in order of increasing energy: microwave, UV, visible, and IR.

Answer: microwave < IR < visible < UV

1

67) Arrange the following regions of the electromagnetic spectrum in order of increasing wavelength: X-ray, radio, UV, and IR.

Answer: X-ray < UV < IR < radio

1

68) What wavenumber corresponds to the wavelength of 4  $\mu\text{m}$ ?

Answer: 2500  $\text{cm}^{-1}$

2

69) Rank the following bonds in order of increasing stretching frequency ( $\text{cm}^{-1}$ ) in IR spectroscopy: C-H,  $\text{C}\equiv\text{C}$ , C-O, and C=O.

Answer:  $\text{C-O} < \text{C=O} < \text{C}\equiv\text{C} < \text{C-H}$

2

70) Rank the following bonds in order of increasing stretching frequency ( $\text{cm}^{-1}$ ) in IR spectroscopy:

C-H,  $\text{C}\equiv\text{N}$ , C-N, and C=O.

Answer:  $\text{C-N} < \text{C=O} < \text{C}\equiv\text{N} < \text{O-H}$

2

71) Which of the following most closely matches the  $\text{C}\equiv\text{C}$  stretching frequency?

A) 3300

B) 3000

C) 2200

D) 1700

E) 1200

Answer: C

2

72) Which of the following has a C-H stretch that occurs at the highest stretching frequency?

A) hexane

B) hex-1-ene

C) (*E*)-hex-2-ene

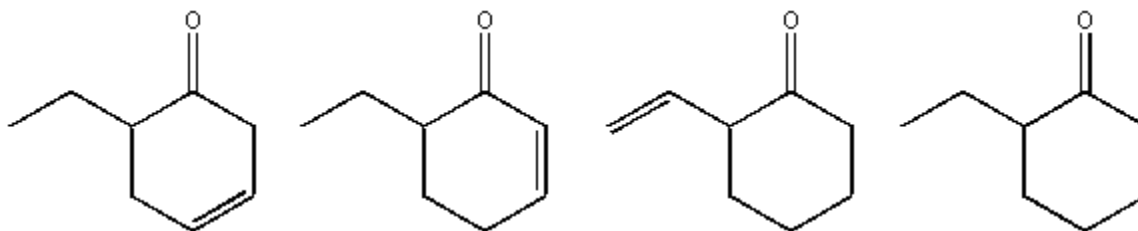
D) hex-1-yne

E) hex-2-yne

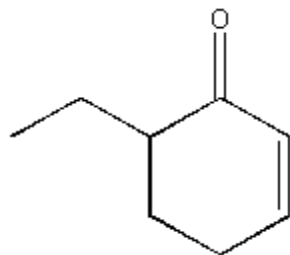
Answer: D

2

73) Which of the following compounds has the lowest carbonyl stretching frequency?



Answer:



2

74) What  $m/z$  characterizes a strong peak in the mass spectrum of cyclopentanol?

- A) 86
- B) 85
- C) 84
- D) 70
- E) 68

Answer: E

2

75) The presence of which element is indicated by a peak at  $m/z$  127 and a characteristic 127-unit gap in the mass spectrum?

- A) Br
- B) Cl
- C) I
- D) N
- E) S

Answer: C

1

76) What wavelength in mm is equivalent to a wavenumber of  $1750\text{ cm}^{-1}$ ?

Answer: 5.71 mm

2

77) Which of the following molecules would be expected to have its C=C stretching frequency at the highest wavenumber: benzene, 1,3-pentadiene, or 1-pentene?

Answer: 1-pentene

2

78) Which of the following would not have a C-H stretch at about  $3050\text{ cm}^{-1}$ ?

- A) 1-pentene
- B) 2-pentene
- C) 2-methyl-2-pentene
- D) 2,3-dimethyl-2-pentene
- E) 2,4-dimethyl-2-pentene

Answer: D

2

79) Which of the following stretches tends to be the least intense?

- A) O-H (alcohol)
- B) O-H (carboxylic acid)
- C) C-H
- D) C=O
- E) C=C

Answer: E

2

80) Which of the following compounds would contain characteristic IR stretches at  $3300$  and  $2200\text{ cm}^{-1}$ ?

- A)  $\text{CH}_3\text{CH}_2\text{CHO}$
- B)  $\text{CH}_3\text{CH}=\text{CHCH}_2\text{OH}$
- C)  $(\text{CH}_3)_2\text{CHCN}$
- D)  $\text{CH}_3\text{CH}_2\text{CH}_2\text{C}\equiv\text{CH}$
- E)  $\text{CH}_3\text{C}\equiv\text{CCH}_2\text{CH}_3$

Answer: D

2

81) Which of the following does not have a broad absorption with one or more spikes that is centered about  $3300\text{ cm}^{-1}$  in the IR?

- A)  $(\text{CH}_3\text{CH}_2\text{CH}_2)_3\text{N}$
- B)  $(\text{CH}_3\text{CH}_2\text{CH}_2)_2\text{NH}$
- C)  $\text{CH}_3\text{CH}_2\text{CH}_2\text{NH}_2$
- D)  $(\text{CH}_3)_3\text{CNH}_2$
- E)  $(\text{CH}_2=\text{CHCH}_2)_2\text{NH}$

Answer: A

2

82) In addition to a carbonyl stretch, which of the following molecules exhibits two characteristic stretches at  $2700$  and  $2800\text{ cm}^{-1}$ ?

- A)  $(\text{CH}_3\text{CH}_2)_2\text{CO}$
- B)  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CHO}$
- C)  $\text{CH}_3\text{CH}_2\text{CO}_2\text{CH}_3$
- D)  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CO}_2\text{H}$
- E)  $\text{CH}_3\text{CH}_2\text{CH}_2\text{COCl}$

Answer: B

2

83) Which of the following molecules would have the highest frequency carbonyl stretch?

- A)  $(\text{CH}_3\text{CH}_2)_2\text{CO}$
- B)  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CHO}$
- C)  $\text{CH}_3\text{CH}_2\text{CO}_2\text{CH}_3$
- D)  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CO}_2\text{H}$
- E)  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CONH}_2$

Answer: C

2

84) Which of the following bonds, C–N, C=N, or C≡N, has an IR stretch around  $1600\text{ cm}^{-1}$ ?

Answer: C=N

2

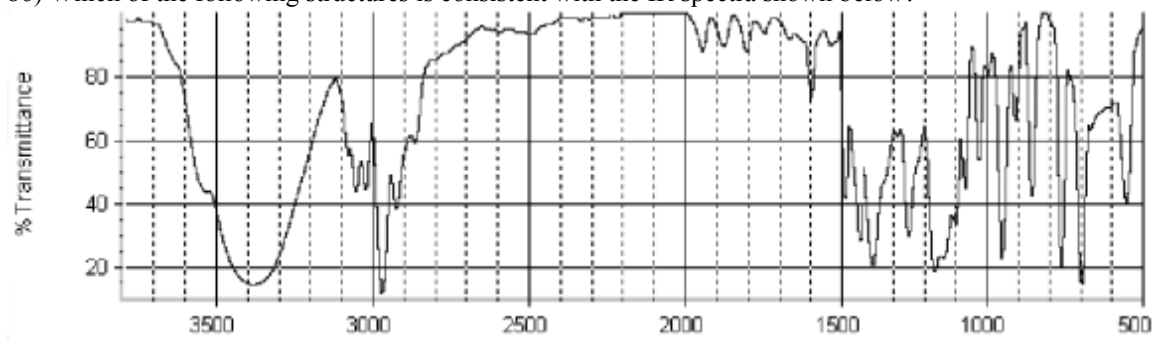
85) Arrange the following IR bond stretches in order of increasing wavenumber:

C≡O, C≡C, O–H, and C=C.

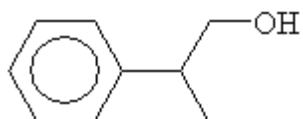
Answer: C–O < C=C < C≡C < O–H

2

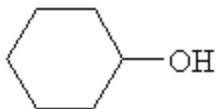
86) Which of the following structures is consistent with the IR spectra shown below?



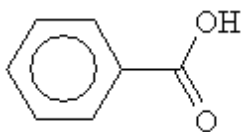
A)



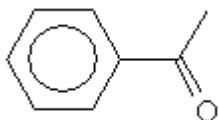
B)



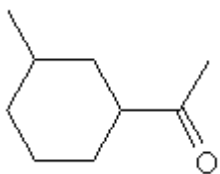
C)



D)



E)



Answer: A

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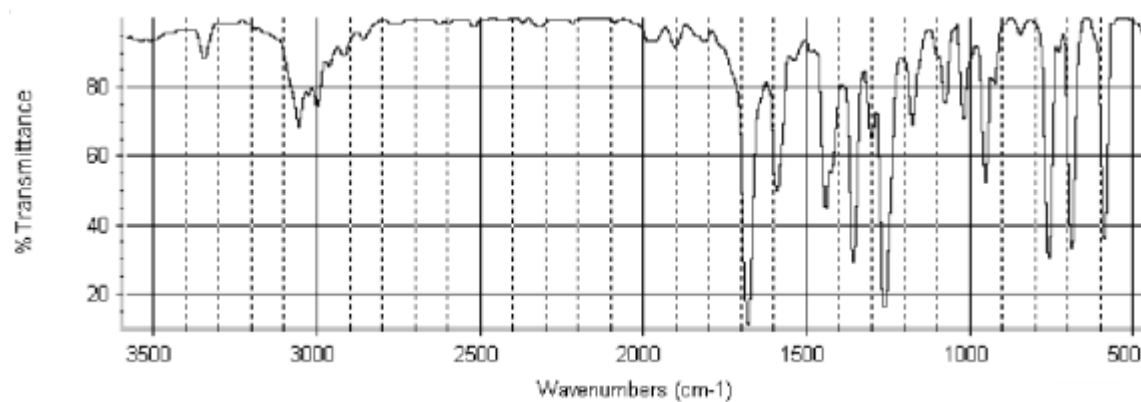
87) One of the following functional groups, sometimes shows a single weak to medium IR adsorption peak in the 2100 to 2250  $\text{cm}^{-1}$  range. Depending on the structure of the compound this peak is sometimes not present, making it easy to misinterpret the spectrum. Which functional group is it?

- A) Carbonyl
- B) Alkyne
- C) Alcohol
- D) Alkene
- E) Carboxylic acid

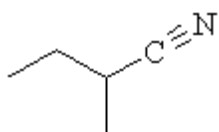
Answer: B

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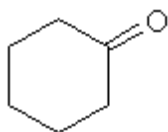
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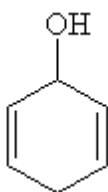
A)



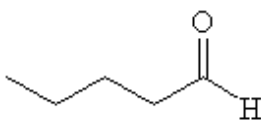
B)



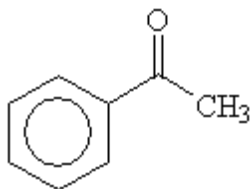
C)



D)



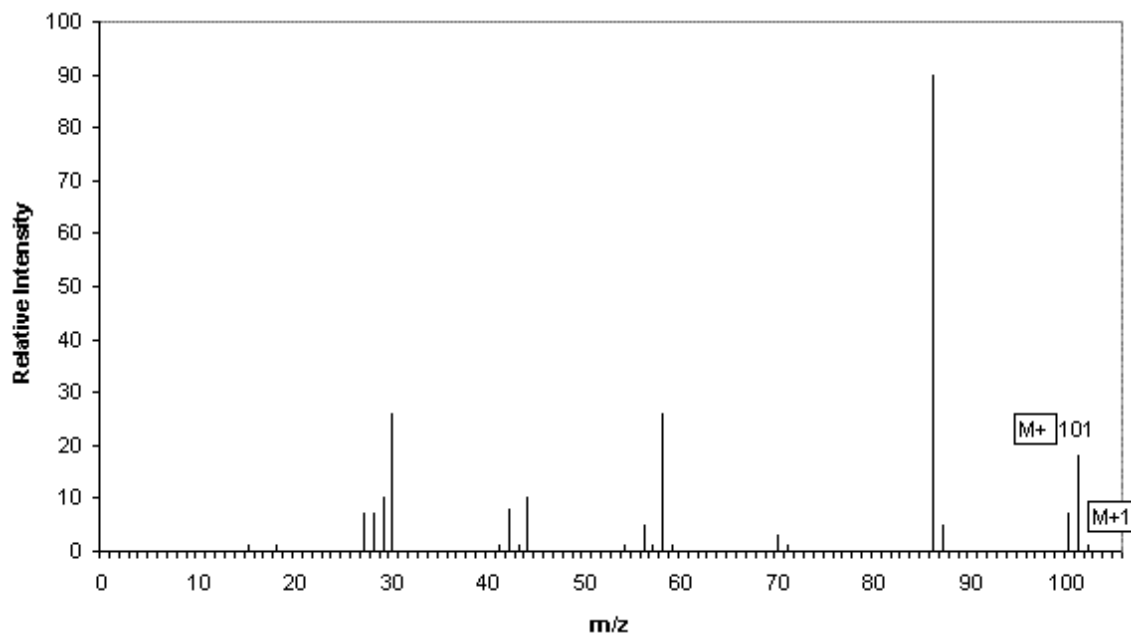
E)



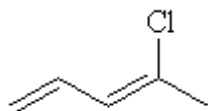
Answer: E

3

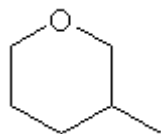
89) Which of the following structures is consistent with the mass spectrum shown below?



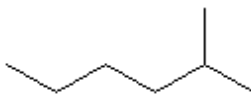
A)



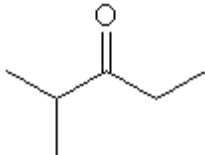
B)



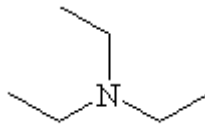
C)



D)



E)



Answer: E

2

90) What are the predicted  $m/z$  values (masses) and relative heights of all the molecular ions of 1-bromoethane that would appear on a mass spectrum (excluding peaks produced by  $^{13}\text{C}$  and  $^2\text{H}$ )?

A)  $M^+$  peak at  $m/z = 108$  and an  $M+1$  peak at  $m/z = 110$

The  $M+1$  peak is approximately  $1/2$  the height of the  $M^+$  peak.

B)  $M^+$  peak at  $m/z = 79$  and an  $M+1$  peak at  $81$

The  $M+1$  peak is approximately the same height as the  $M^+$  peak.

C)  $M^+$  peak at  $m/z = 108$  and an  $M+2$  peak at  $m/z = 110$

The  $M+2$  peak is approximately the same height as the  $M^+$  peak.

D)  $M^+$  peak at  $m/z = 108$  and an  $M+2$  peak at  $m/z = 110$

$M+2$  peak is approximately  $1/2$  the height of the  $M^+$  peak.

E)  $M^+$  peak at  $m/z = 79$  and an  $M+1$  peak at  $81$

The  $M+1$  peak is approximately  $1/2$  the height of the  $M^+$  peak.

Answer: C

2