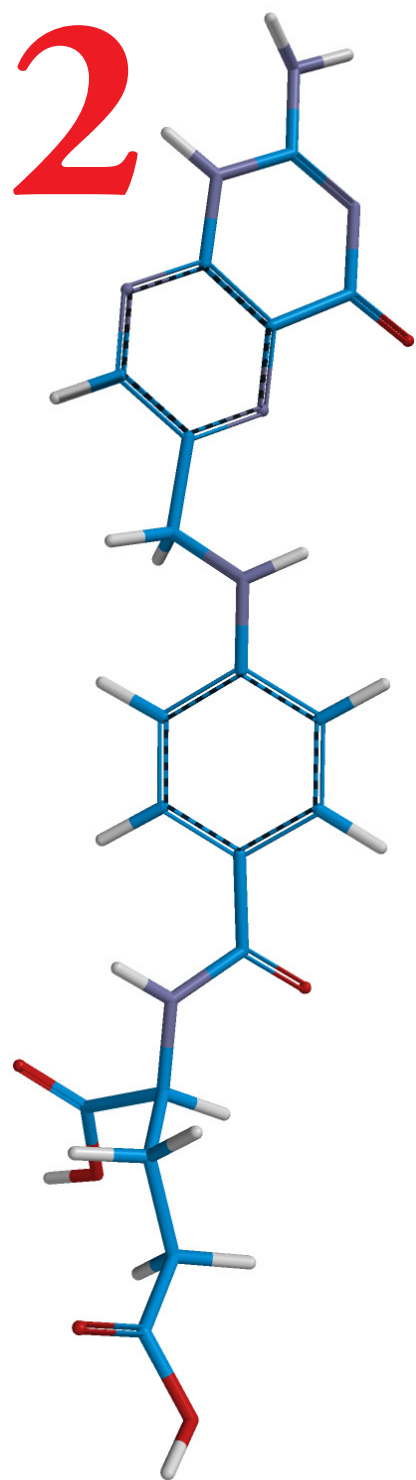


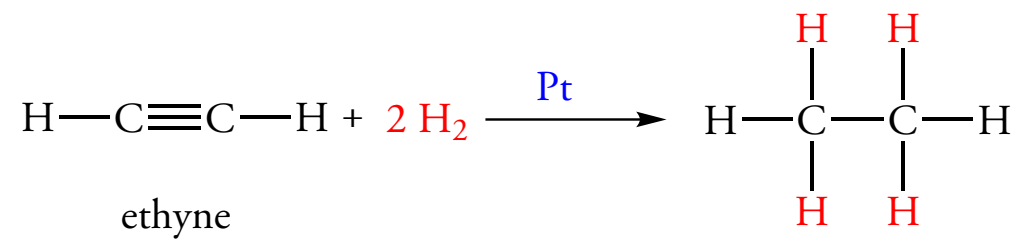
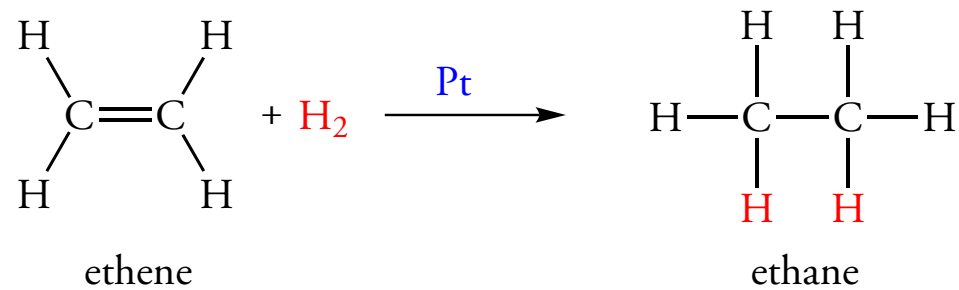
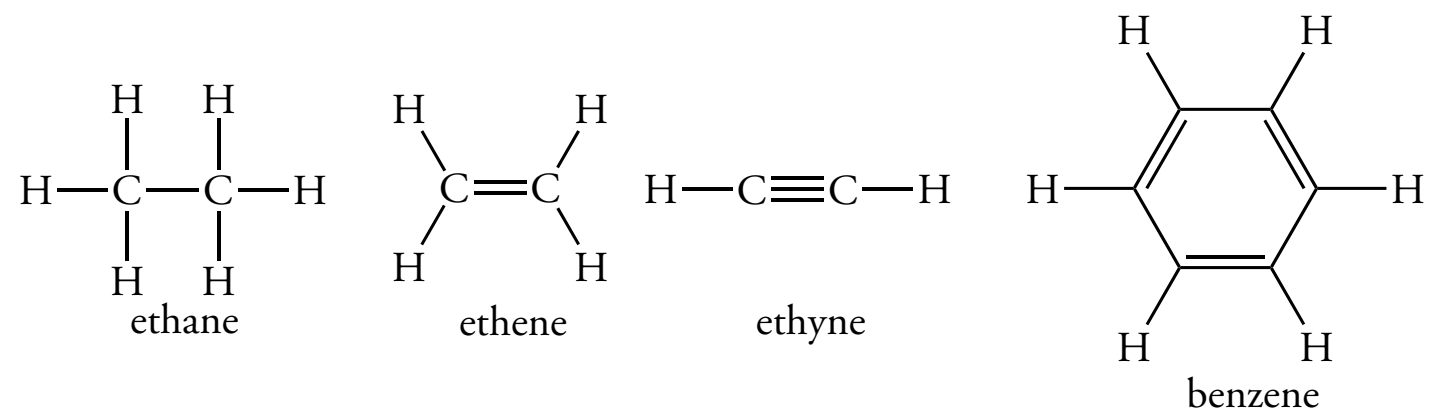
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PART I: FUNCTIONAL GROUPS AND THEIR PROPERTIES

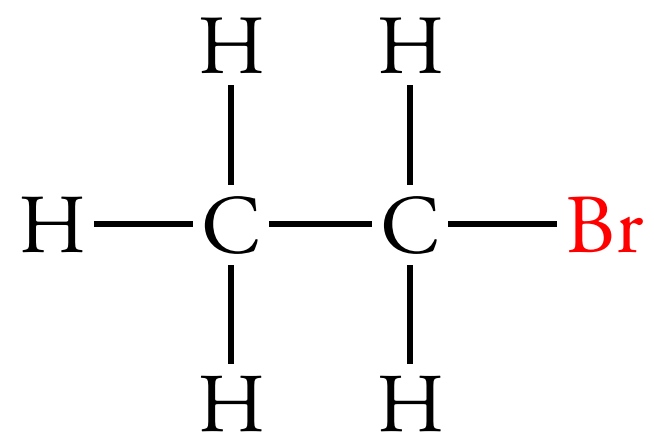
2.1 INTRODUCTION TO FUNCTIONAL GROUPS: HYDROCARBONS AND HALOALKANES

Hydrocarbons



2.1 INTRODUCTION TO FUNCTIONAL GROUPS: HYDROCARBONS AND HALOALKANES

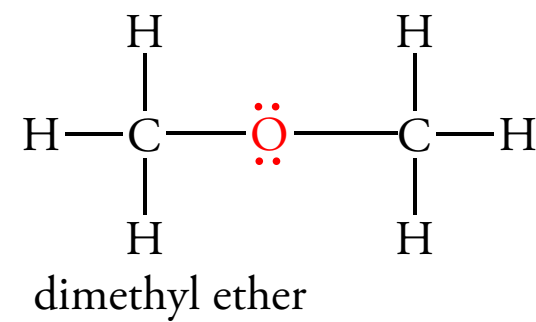
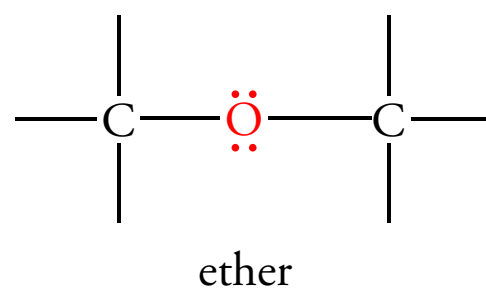
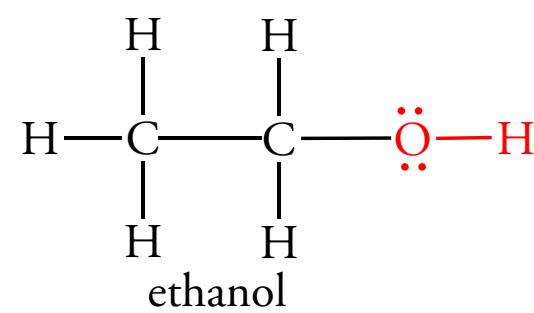
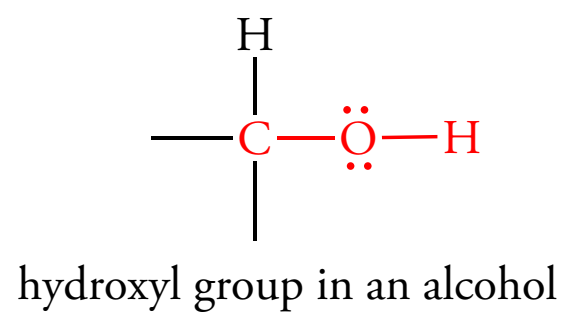
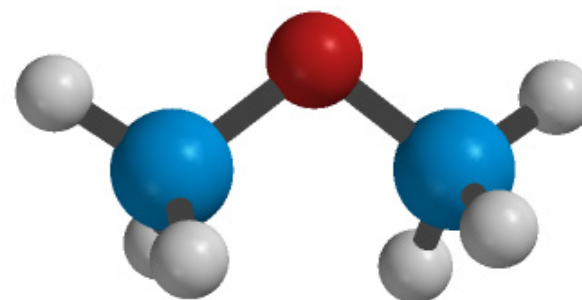
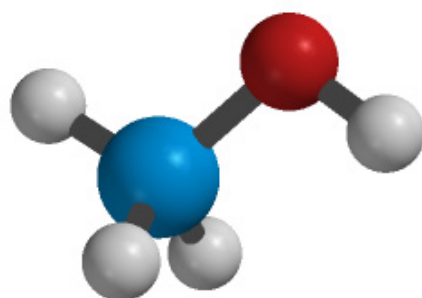
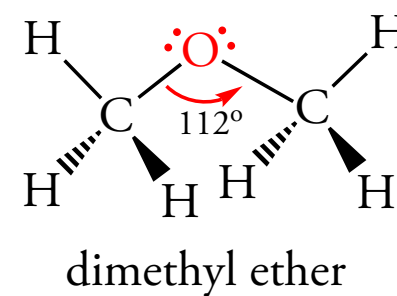
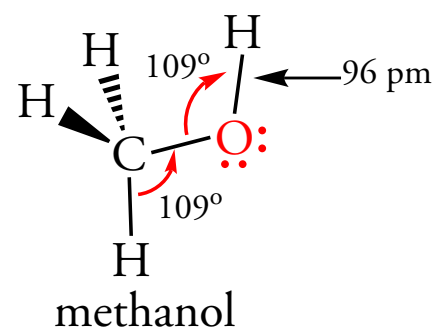
Haloalkanes



bromoethane, a haloalkane

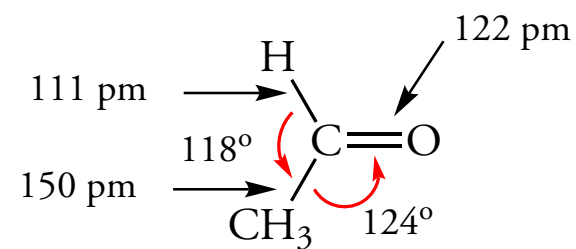
2.2 FUNCTIONAL GROUPS THAT CONTAIN OXYGEN

Carbon-Oxygen Single Bonds in Alcohols and Ethers

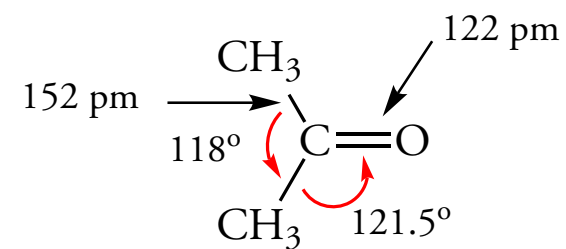
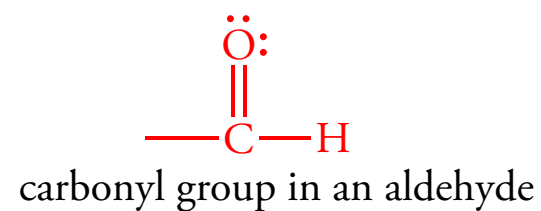
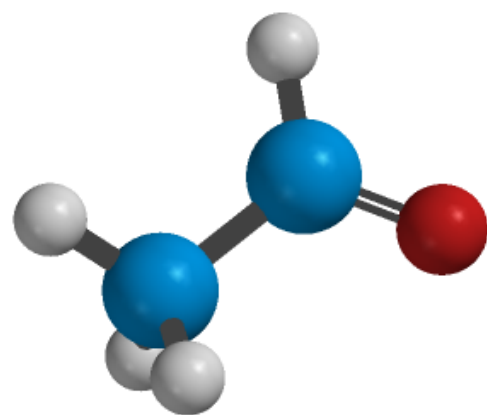


2.2 FUNCTIONAL GROUPS THAT CONTAIN OXYGEN

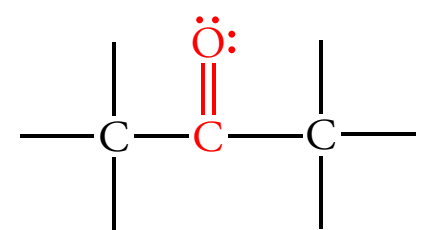
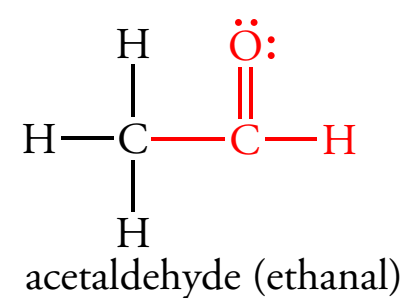
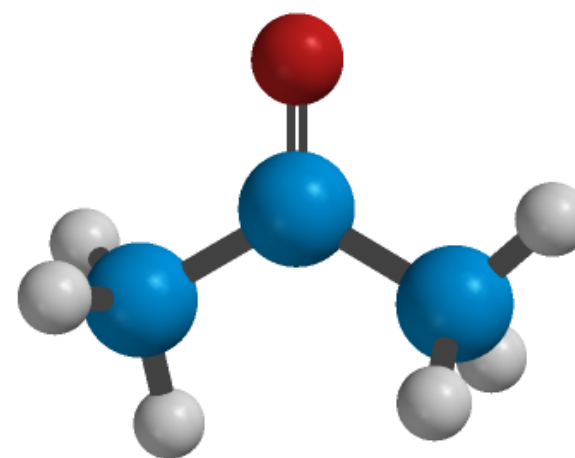
Carbon-Oxygen Double Bonds in Aldehydes and Ketones



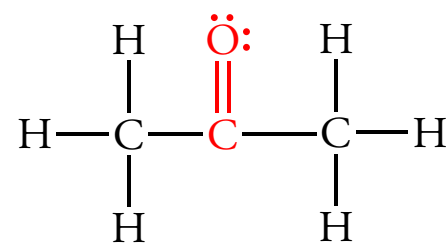
ethanal
(acetaldehyde)



propanone
(acetone)



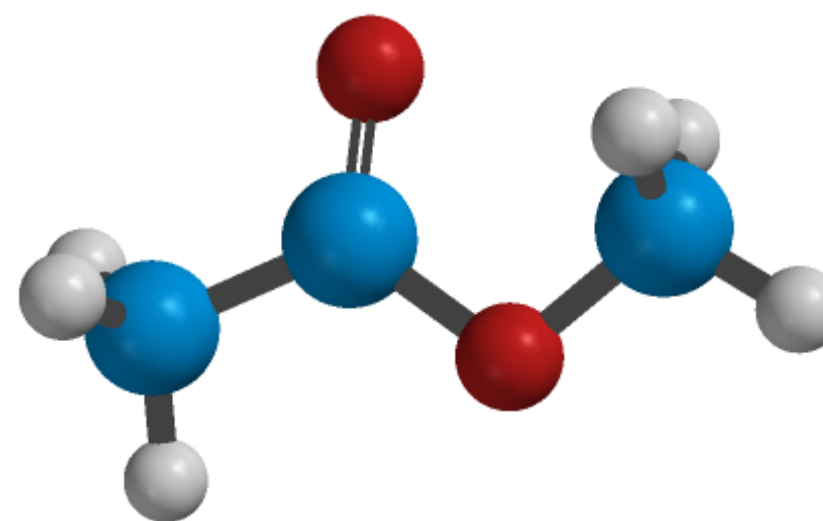
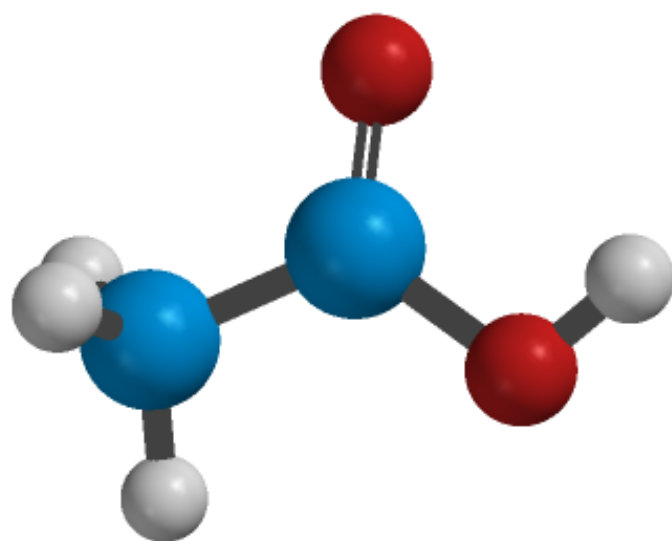
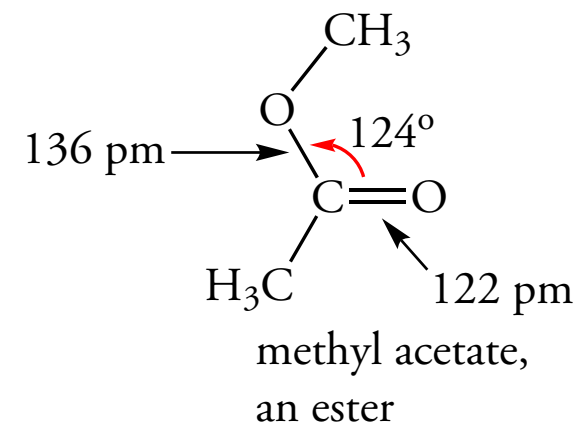
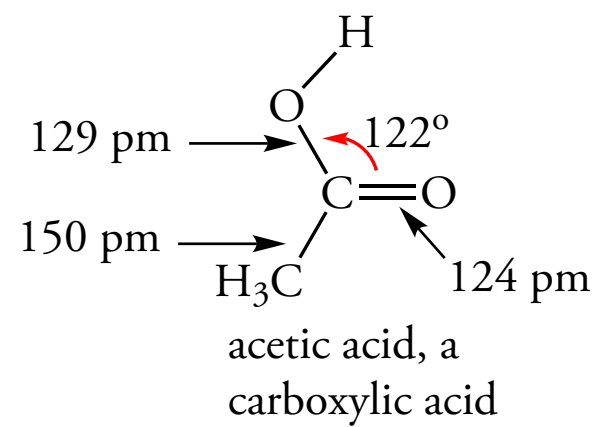
carbonyl group in ketone



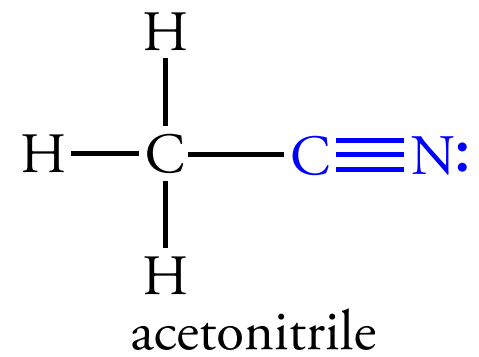
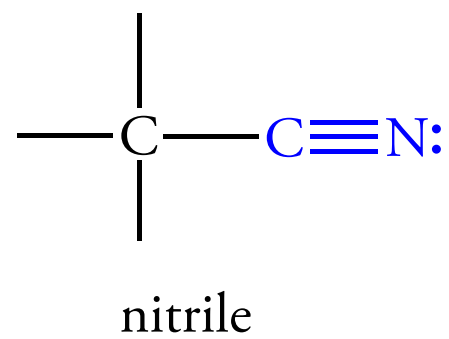
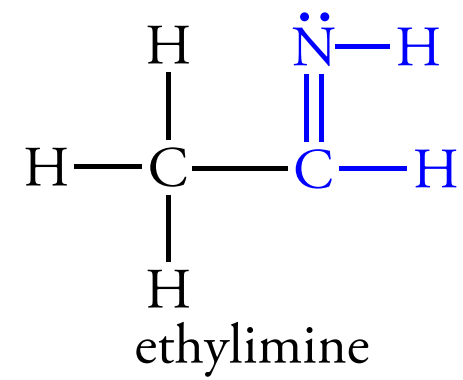
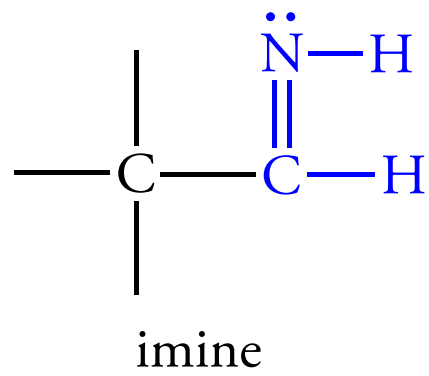
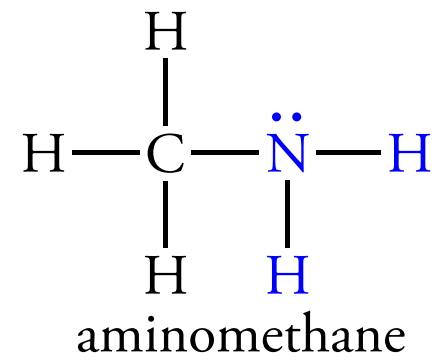
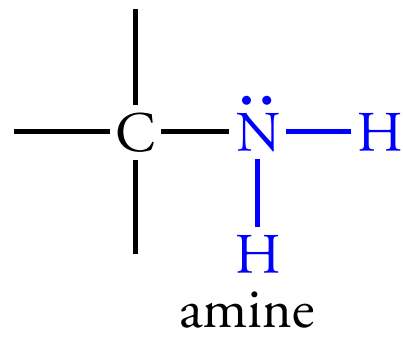
propanone (acetone)

2.2 FUNCTIONAL GROUPS THAT CONTAIN OXYGEN

Carboxylic Acids and Esters

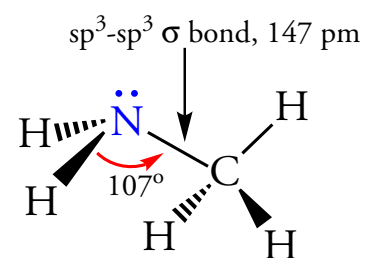


2.3 FUNCTIONAL GROUPS THAT CONTAIN NITROGEN

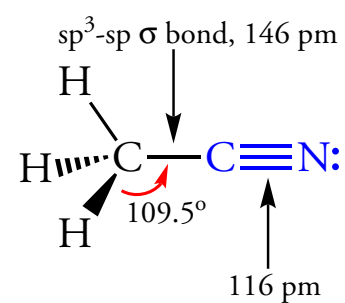


2.3 FUNCTIONAL GROUPS THAT CONTAIN NITROGEN

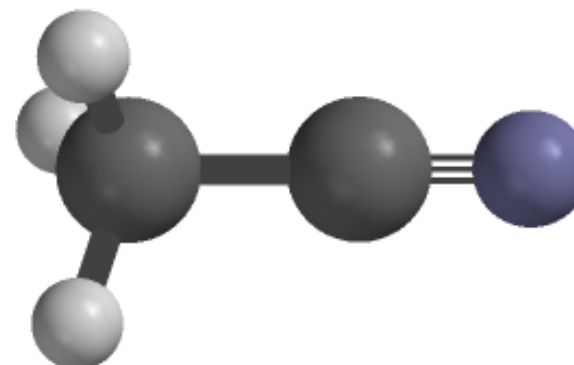
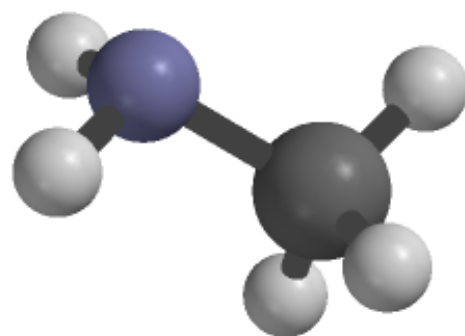
Figure 2.4 Structures of Amines and Nitriles



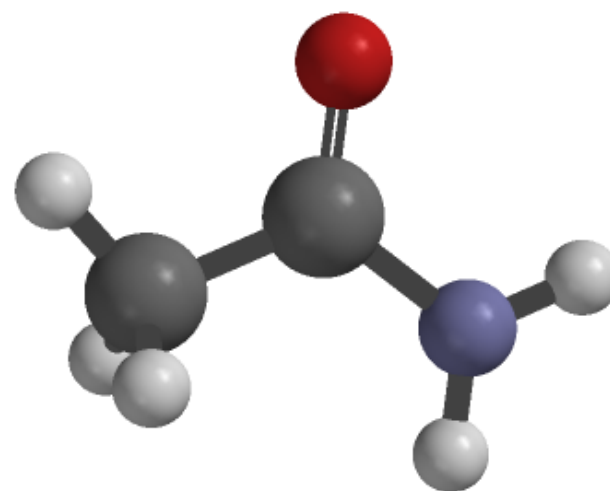
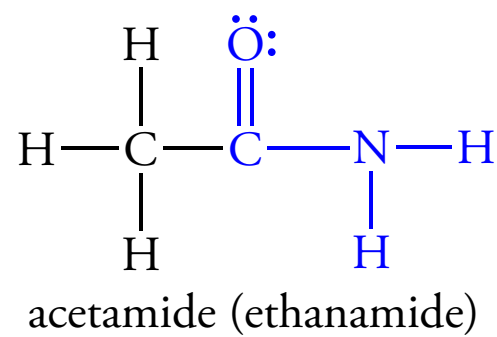
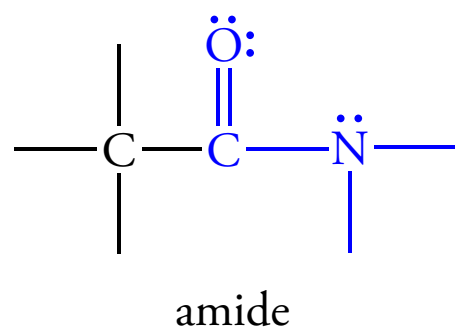
(a) amine bond lengths and bond angles



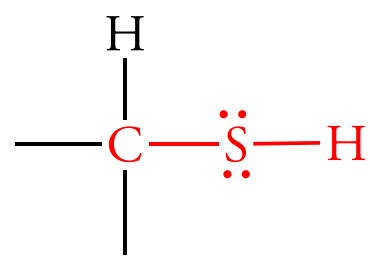
(b) nitrile bond lengths and bond angles



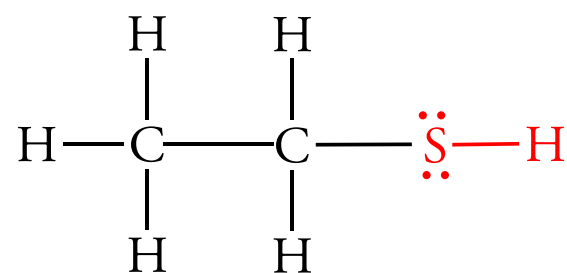
Amides



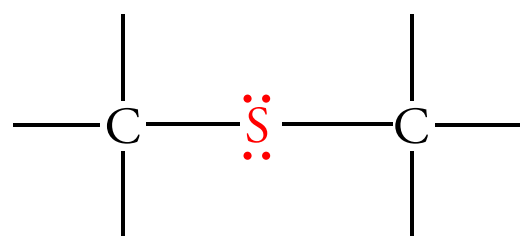
2.4 FUNCTIONAL GROUPS THAT CONTAIN SULFUR



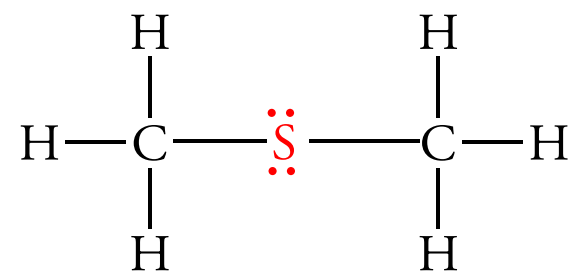
sulphydryl group in a thiol



ethanethiol

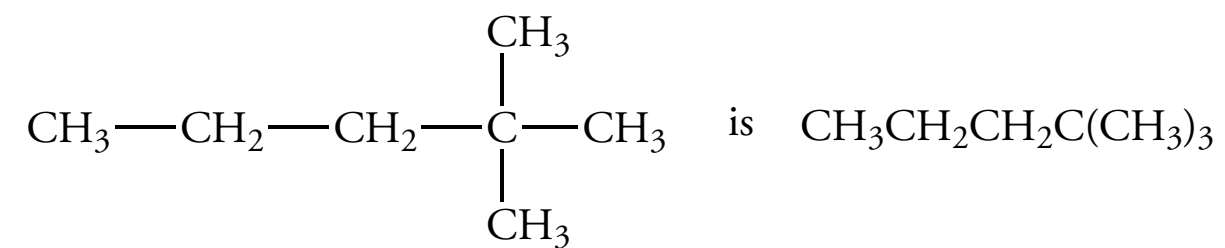
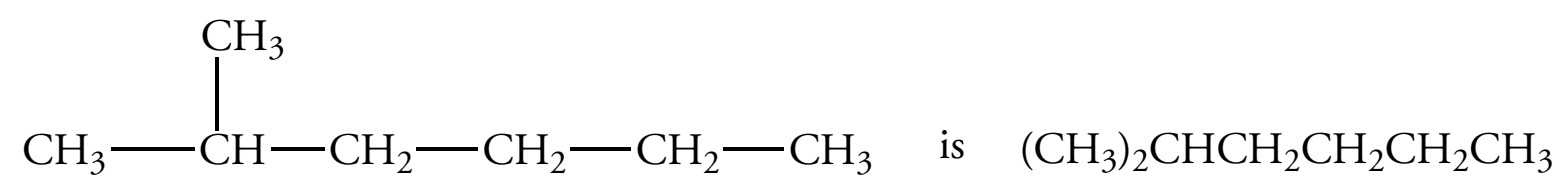
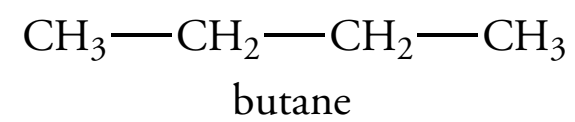


thioether (sulfide)

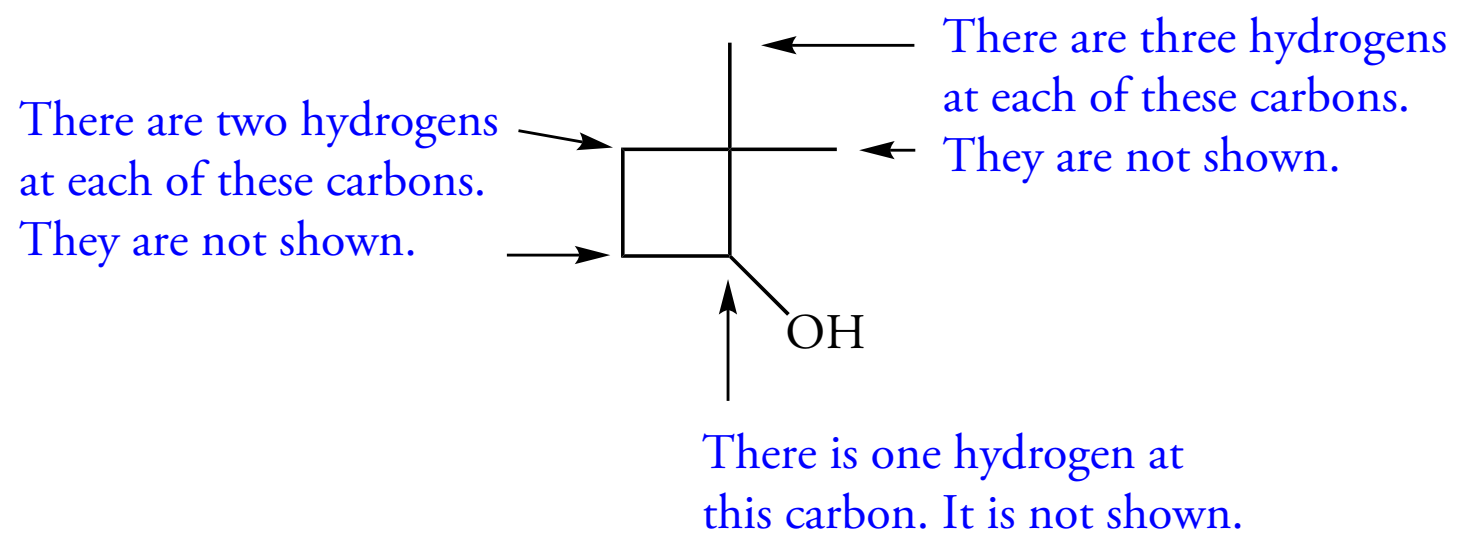
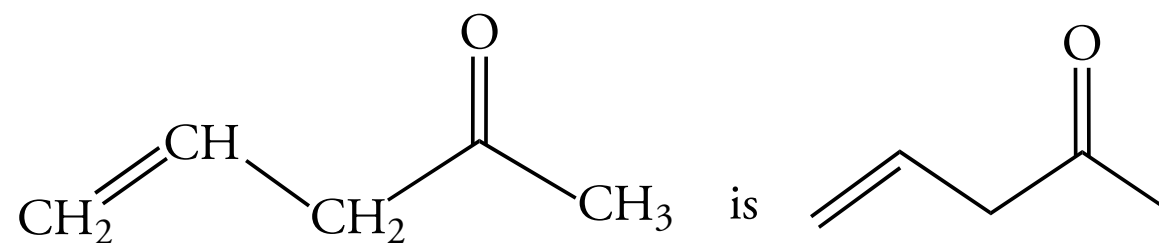
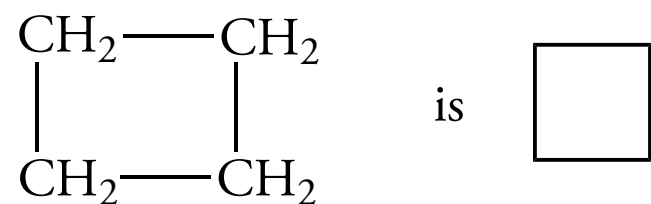
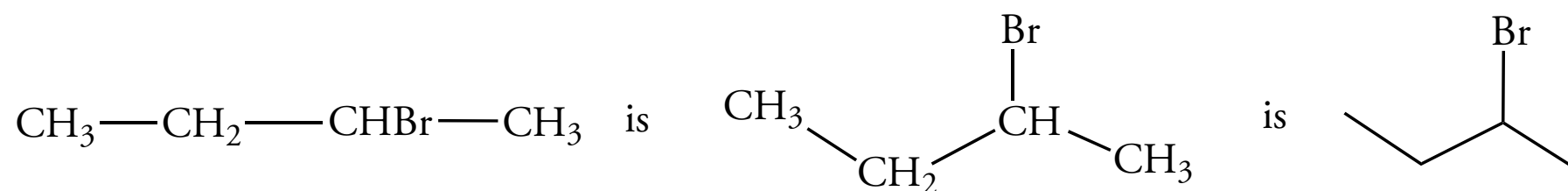


dimethyl sulfide

2.5 STRUCTURAL FORMULAS

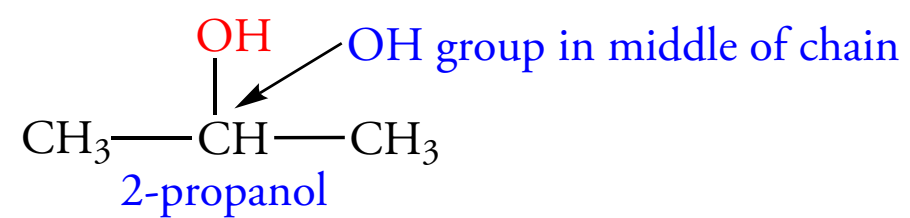
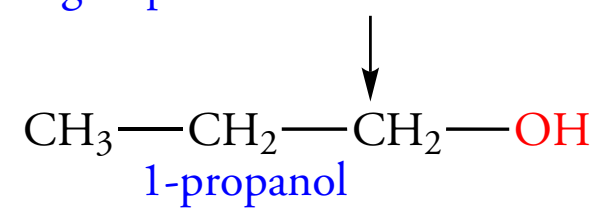


2.6 BOND-LINE STRUCTURES

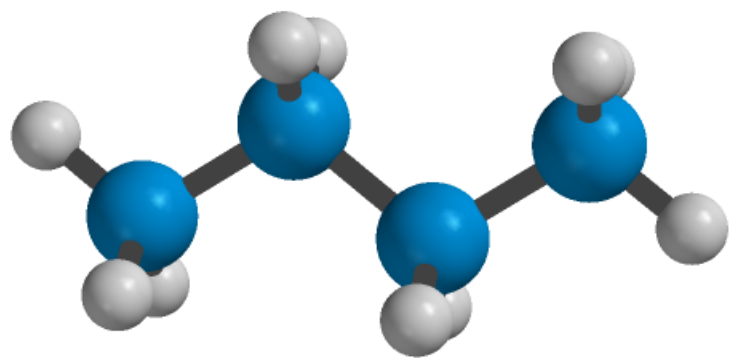


2.7 ISOMERS

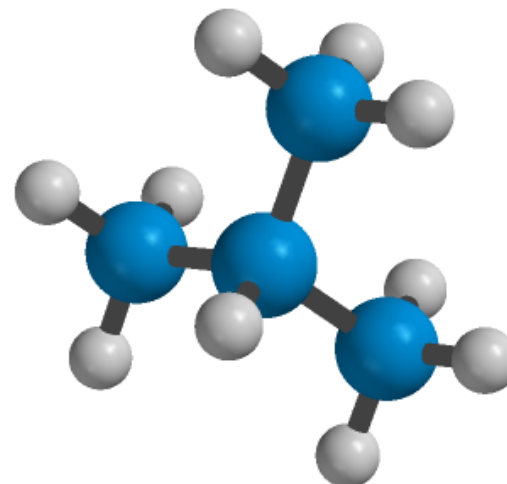
OH group at end of chain



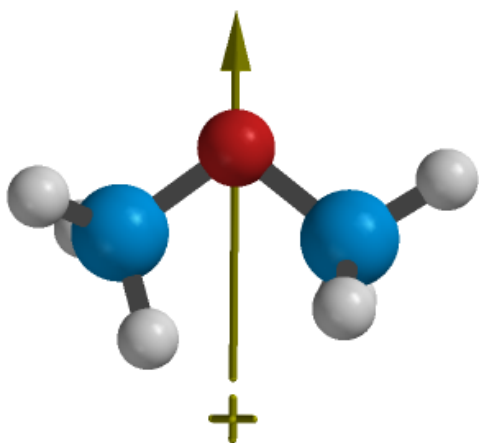
2.7 ISOMERS



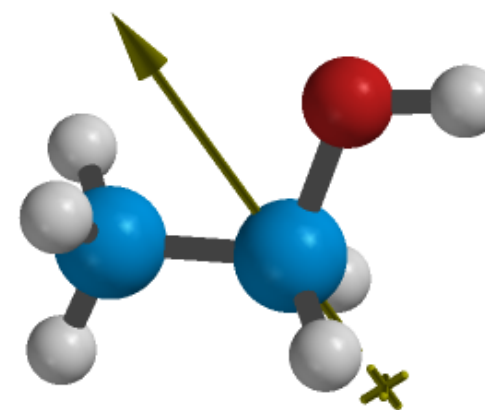
(a)
butane
 $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$
(no branch)



(b)
isobutane
 $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_3$
(branch in middle of chain)



(c)
dimethyl ether
 CH_3OCH_3



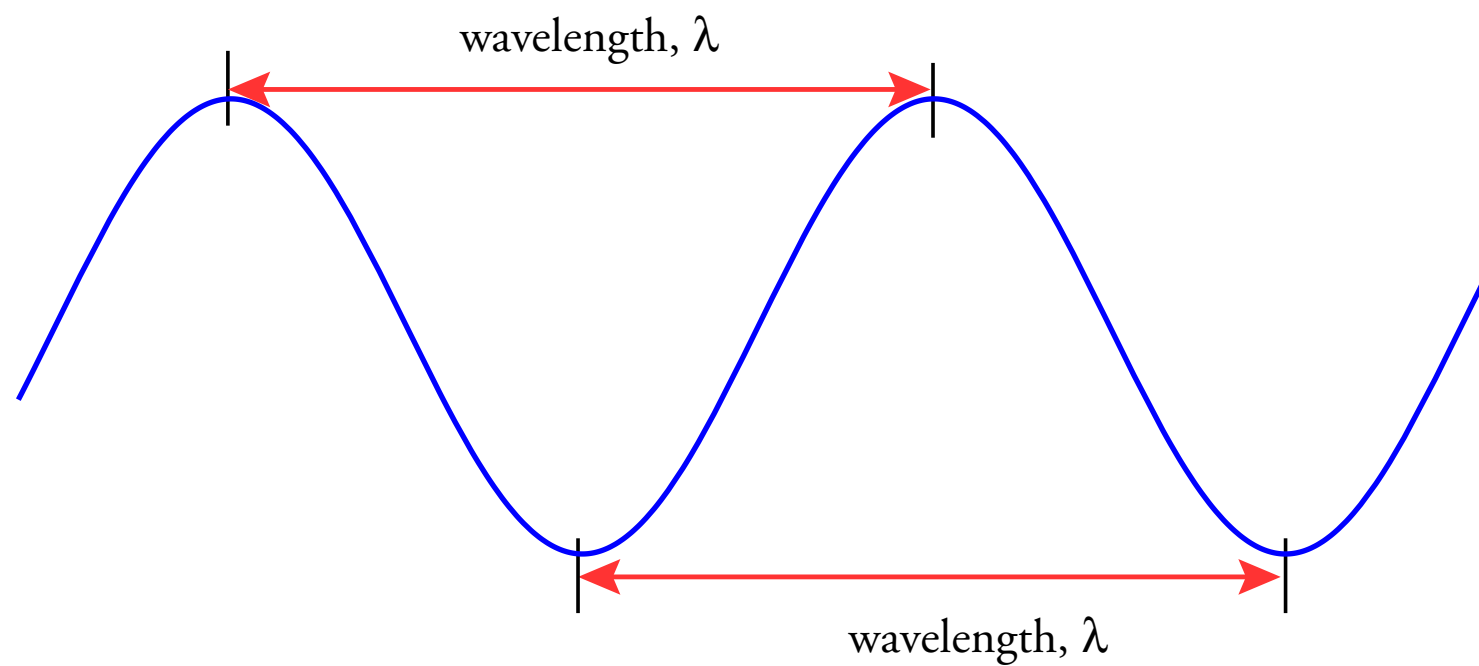
(d)
ethanol
 $\text{CH}_3\text{CH}_2\text{OH}$

**PART II: IDENTIFICATION
OF FUNCTION GROUPS BY
INFRARED SPECTROSCOPY**

2.8 SPECTROSCOPY

Figure 2.6 Electromagnetic Radiation

The wavelength, λ , of electromagnetic radiation is the distance between any two peaks or troughs of the wave.



$$E = h\nu$$

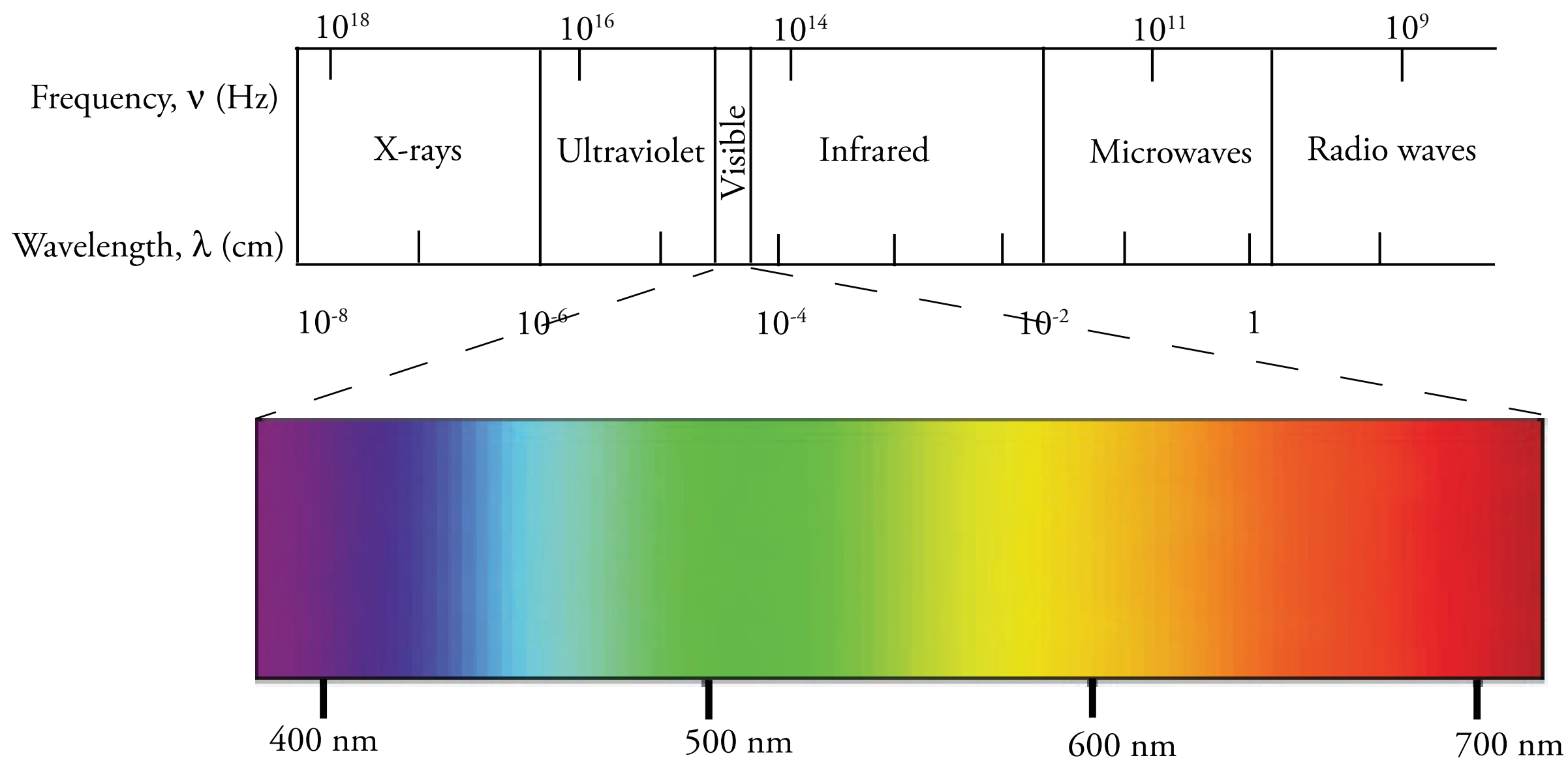
$$E = \frac{hc}{\lambda}$$

$$E = hc \left(\frac{1}{\lambda} \right)$$

2.8 SPECTROSCOPY

Figure 2.7 Electromagnetic Spectrum

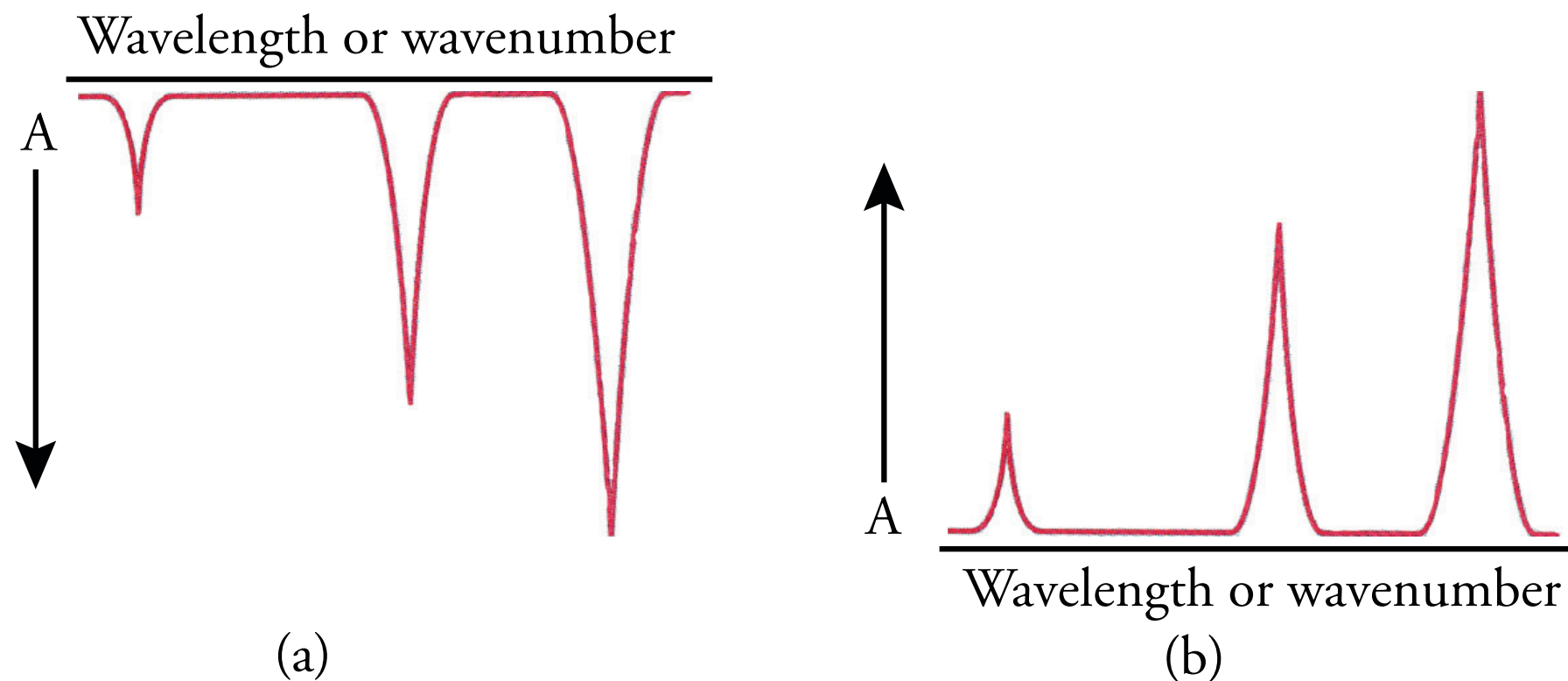
The visible region of the spectrum. The wavelength or the reciprocal of the wavelength, the wavenumber, is used to identify absorptions of organic molecules. The visible spectrum is only a tiny sliver of the entire electromagnetic spectrum,



2.8 SPECTROSCOPY

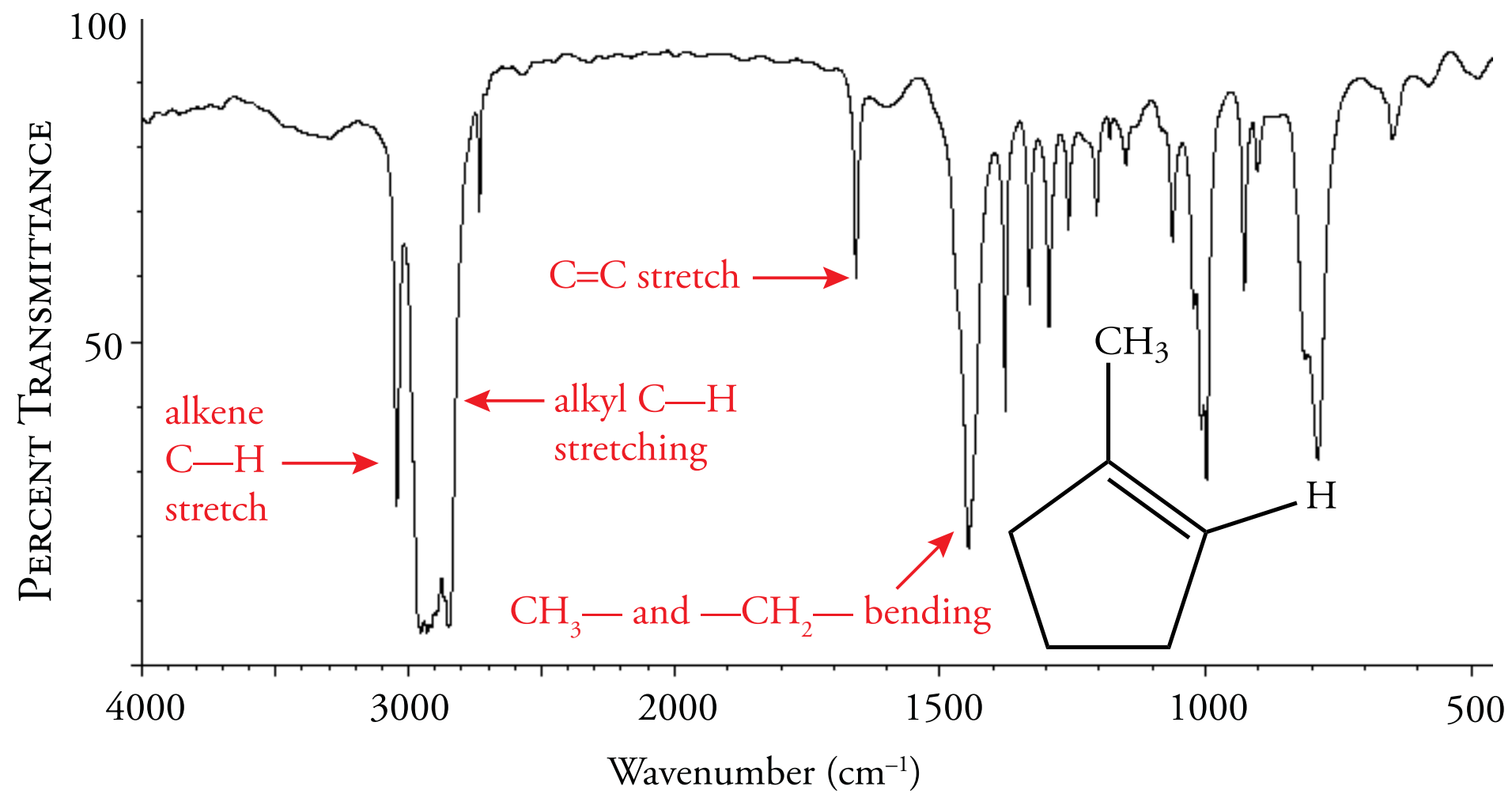
Figure 2.8 Features of a Spectrum

The portion of the spectrum where no absorption occurs is the base line. This horizontal line may be located at the top or bottom of a graph. Absorption then is recorded as a “peak” extending down from the base line. In an infrared spectrum, (a), the base line is at top of the spectrum. In an NMR spectrum, (b), the base line is at the bottom of the spectrum.



2.9 INFRARED SPECTROSCOPY

Figure 2.9 Infrared Spectrum of 1-Methylcyclopentene



2.9 INFRARED SPECTROSCOPY

$$1/\lambda = \frac{1}{2\pi c} \sqrt{\frac{f(m_1 + m_2)}{m_1 m_2}}$$

$$\text{C—C}, \quad \frac{12.0 + 12.0}{12.0 \times 12.0} = 0.17$$

$$\text{C—O}, \quad \frac{12.0 + 16.0}{12.0 \times 16.0} = 0.17$$

$$\text{C—H}, \quad \frac{12.0 + 1.0}{12.0 \times 1.0} = 1.08$$

2.9 INFRARED SPECTROSCOPY

Table 2.1
Approximate Values of Infrared Absorptions

<i>Bond</i>	<i>Absorption region (cm⁻¹)</i>
C—C, C—N, C—O	800-1300
C=C, C=N, C=O	1500-1900
C≡C, C≡N	2000-2300
C—H, N—H, O—H	2850-3650

2.8 SPECTROSCOPY

Table 2.1
Approximate Values of Infrared Absorptions

<i>Bond</i>	<i>Absorption region (cm⁻¹)</i>
C—C, C—N, C—O	800-1300
C=C, C=N, C=O	1500-1900
C≡C, C≡N	2000-2300
C—H, N—H, O—H	2850-3650

Table 2.2

Charateristic Infrared Group Frequencies

<i>Class</i>	<i>Group</i>	<i>Wavenumber (cm⁻¹)</i>
Alkane	C—H	2850-3000
Alkene	C—H	3080-3140
	C=C	1630-1670
Alkyne	C—H	3300-3320
	C≡C	2100-2140
Alcohol	O—H	3400-3600
	C—O	1050-1200
Ether	C—O	1070-1150
Aldehyde	C=O	1725
Ketone	C=O	1700-1780

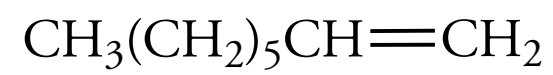
2.10 IDENTIFYING HYDROCARBONS

Table 2.2

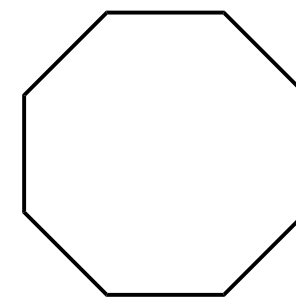
Charateristic Infrared Group Frequencies

<i>Class</i>	<i>Group</i>	<i>Wavenumber (cm⁻¹)</i>
Alkane	C—H	2850-3000
Alkene	C—H	3080-3140
	C=C	1630-1670
Alkyne	C—H	3300-3320
	C≡C	2100-2140
Alcohol	O—H	3400-3600
	C—O	1050-1200
Ether	C—O	1070-1150
Aldehyde	C=O	1725
Ketone	C=O	1700-1780

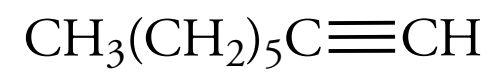
2.10 IDENTIFYING HYDROCARBONS



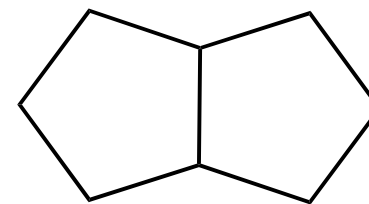
1-octene



cyclooctane



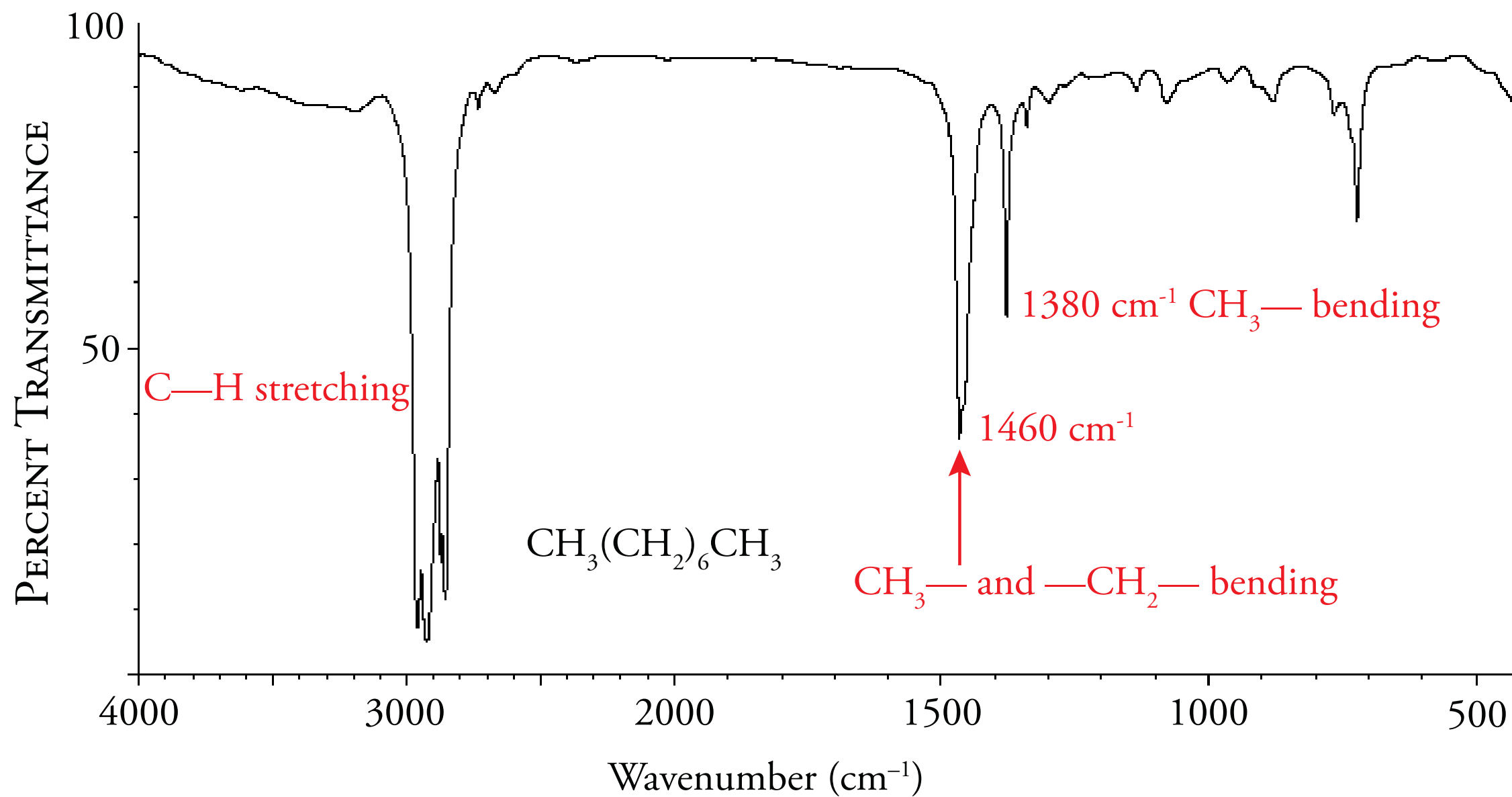
1-octyne



bicyclo[3.3.0]octane

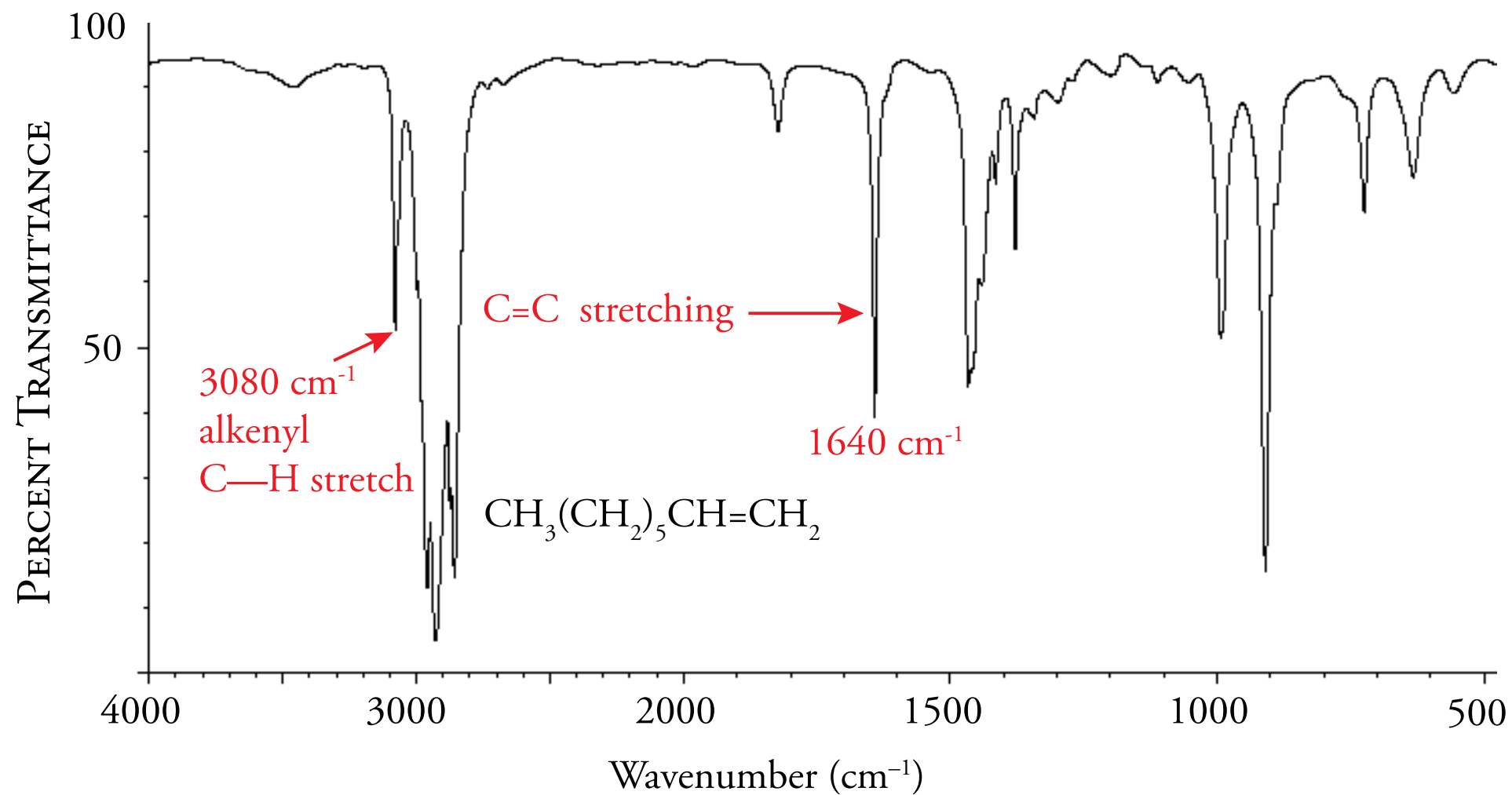
2.10 IDENTIFYING HYDROCARBONS

Figure 2.10a Infrared Spectrum of n-Octane



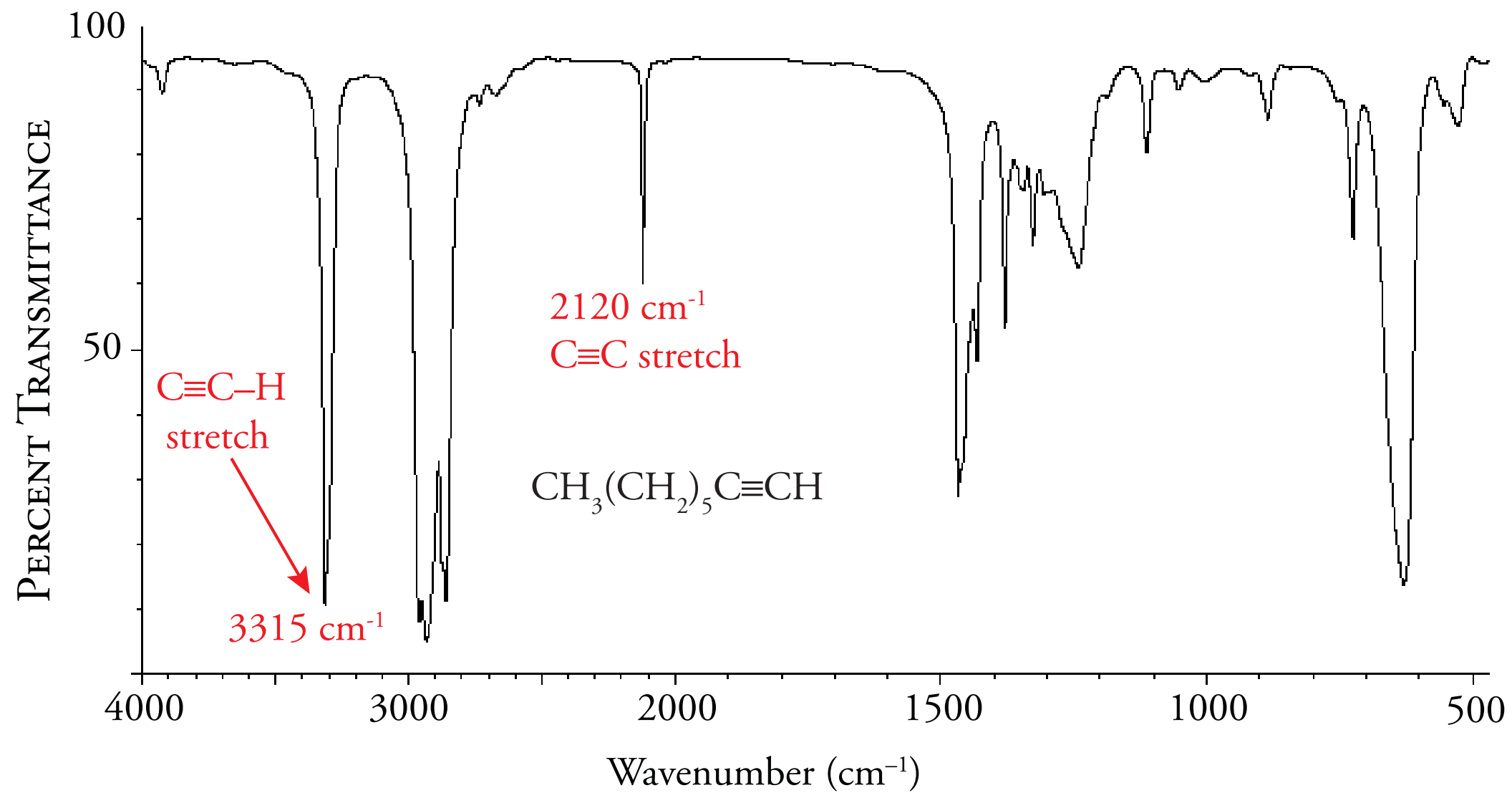
2.10 IDENTIFYING HYDROCARBONS

Figure 2.10b Infrared Spectrum of 1-Octene



2.10 IDENTIFYING HYDROCARBONS

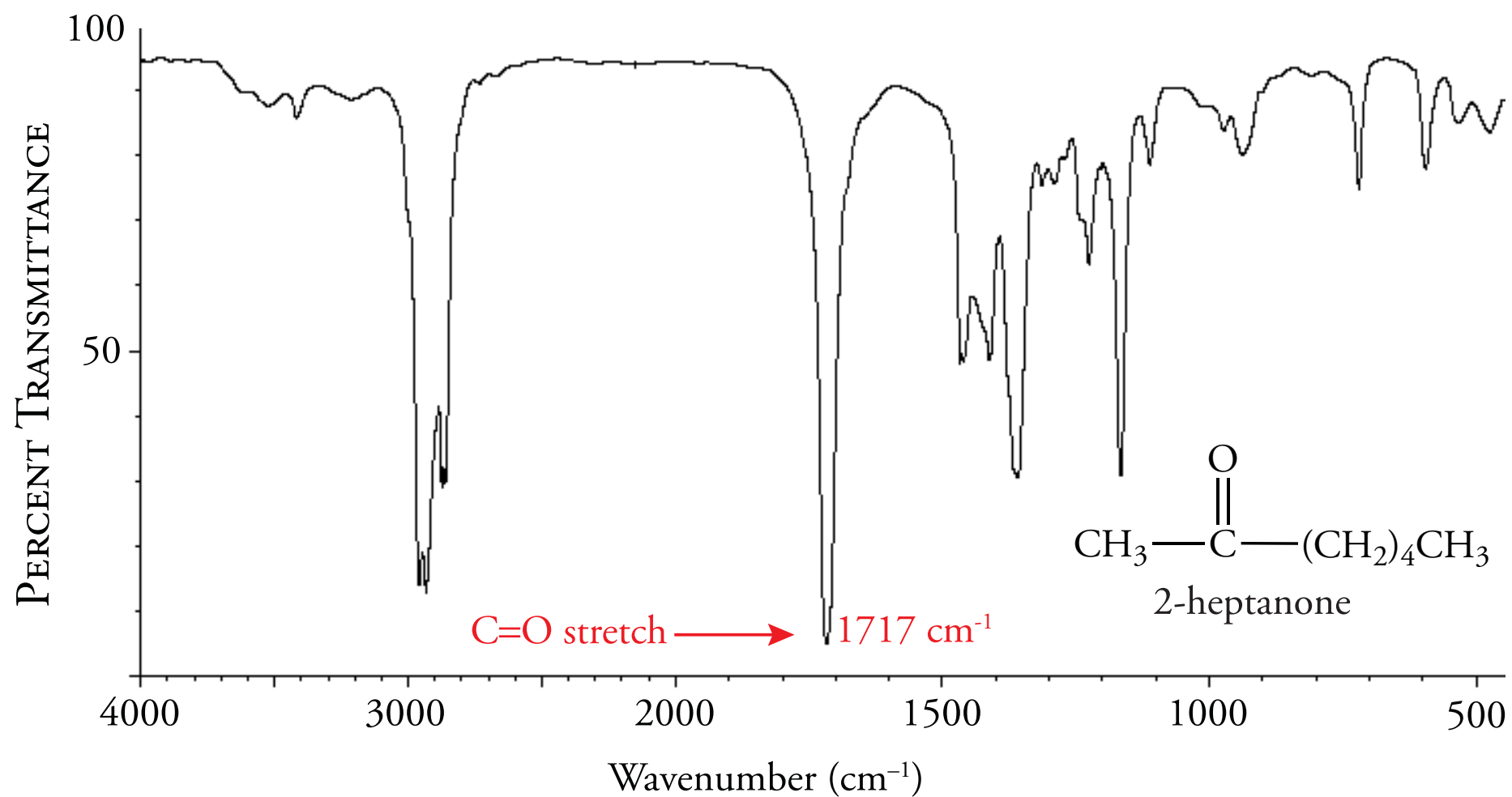
Figure 2.10c Infrared Spectrum of 1-Octyne



2.11 IDENTIFYING OXYGEN-CONTAINING COMPOUNDS

The Carbonyl Group

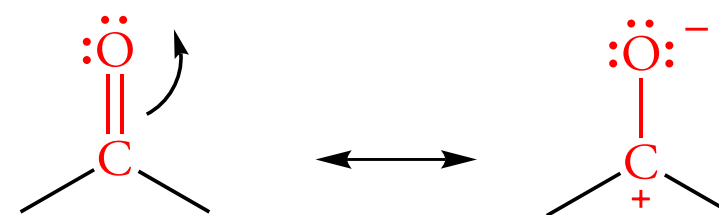
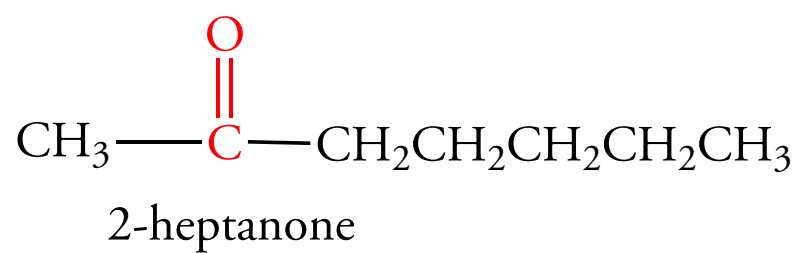
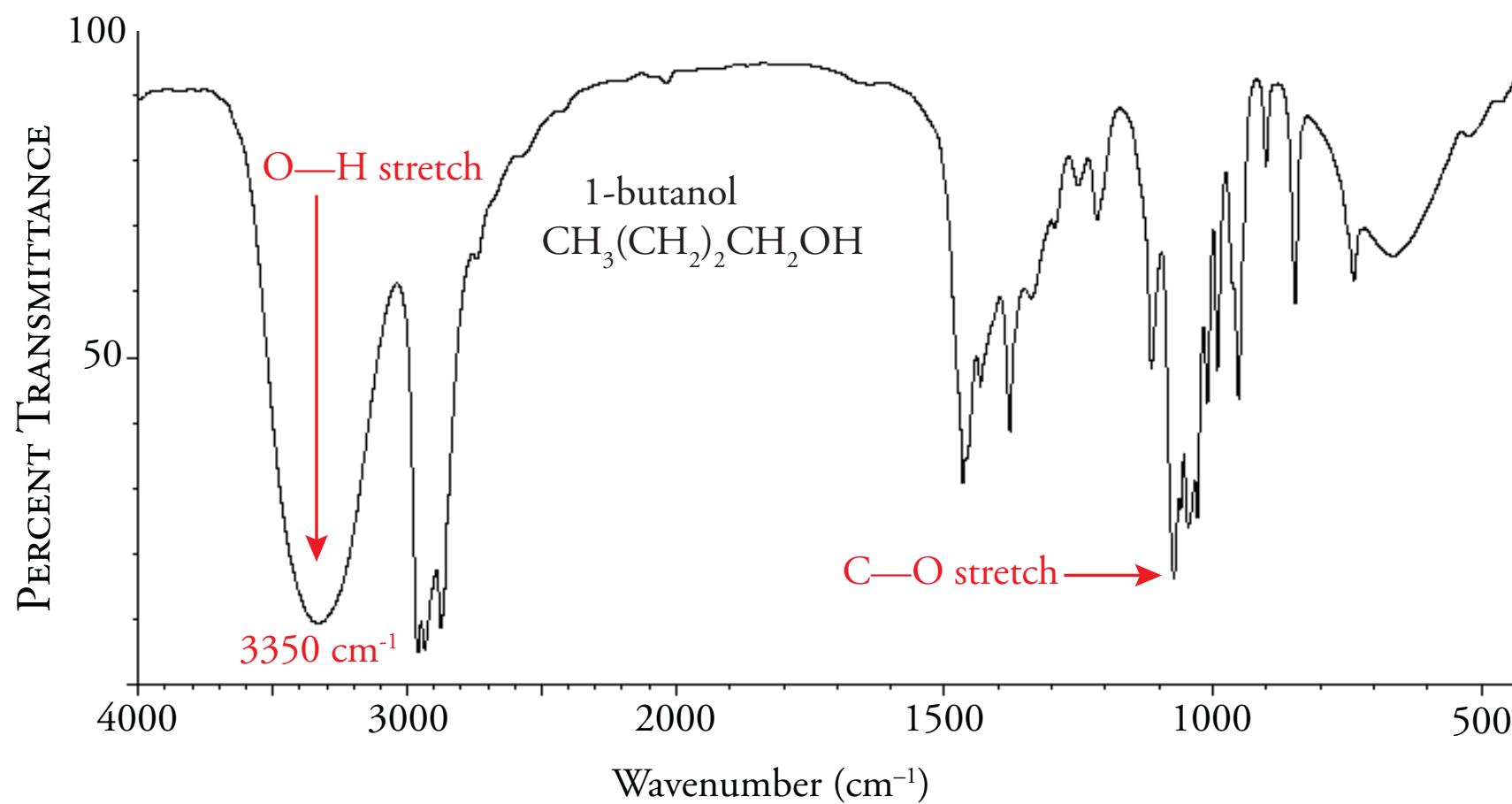
Figure 2.11 Infrared Spectrum of 2-Heptanone



2.11 IDENTIFYING OXYGEN-CONTAINING COMPOUNDS

Alcohols and Ethers

Figure 2.12 Infrared Spectrum of 1-Butanol

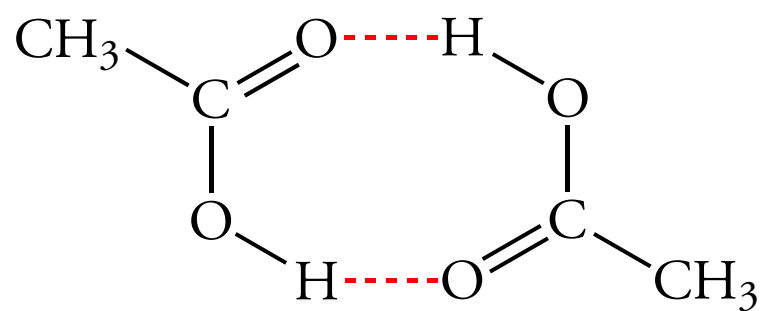
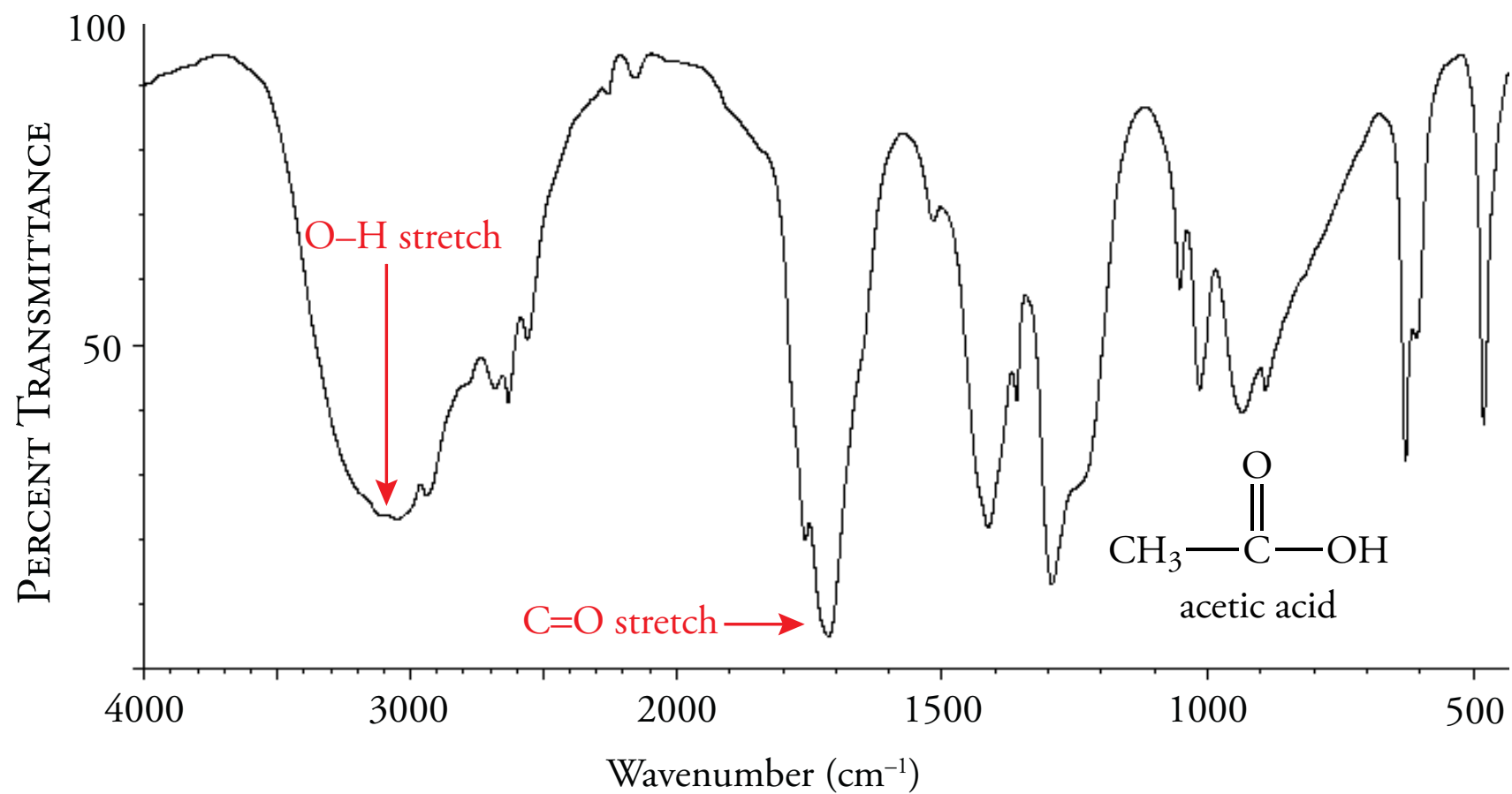


contributing resonance structures of a carbonyl group

2.11 IDENTIFYING OXYGEN-CONTAINING COMPOUNDS

Carboxylic Acids

Figure 2.13 Infrared Spectrum of Acetic Acid

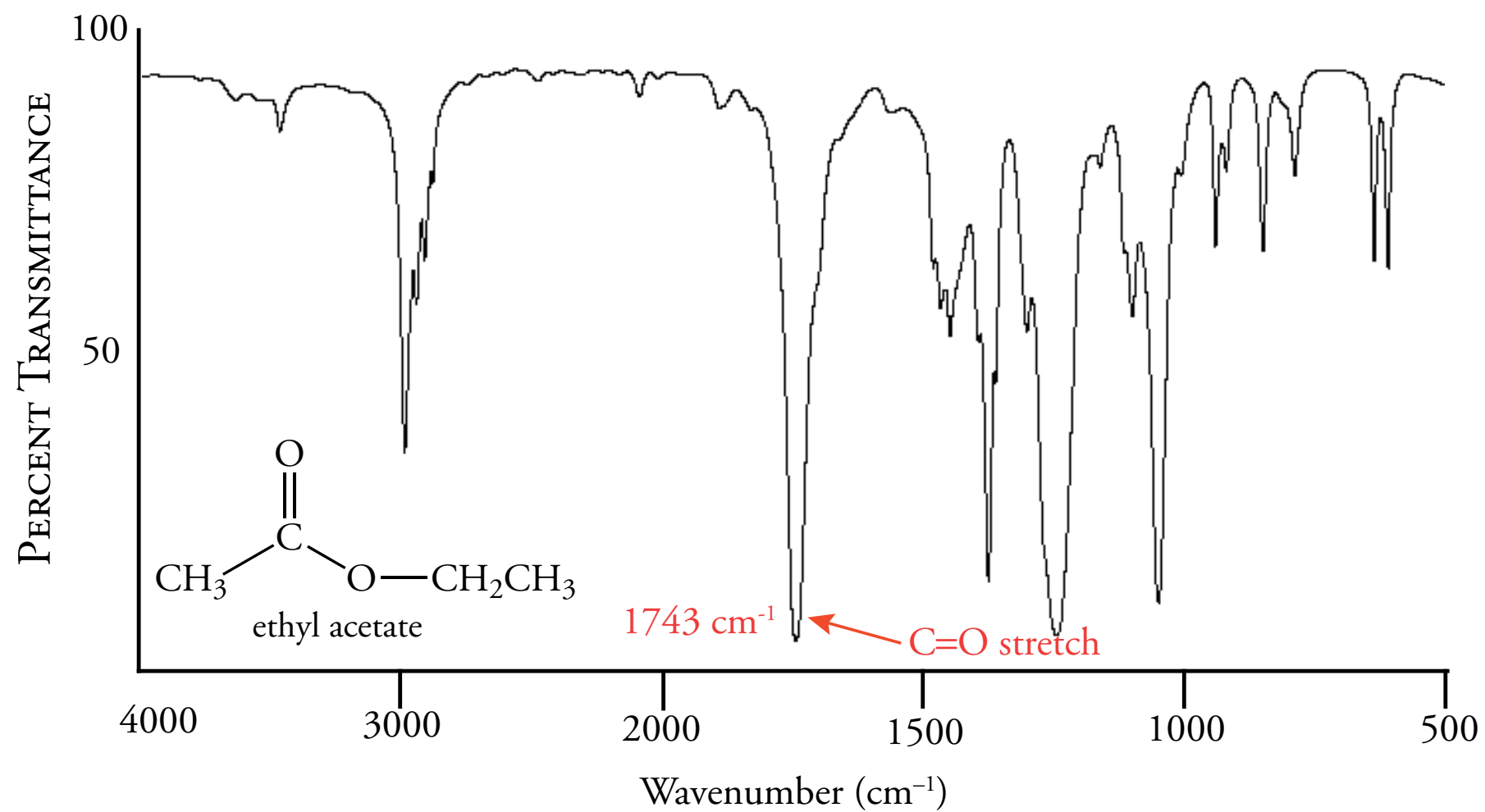


acetic acid, hydrogen-bonded dimer

2.11 IDENTIFYING OXYGEN-CONTAINING COMPOUNDS

Esters

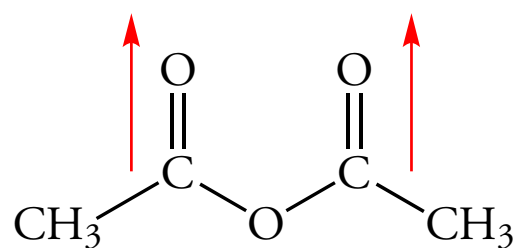
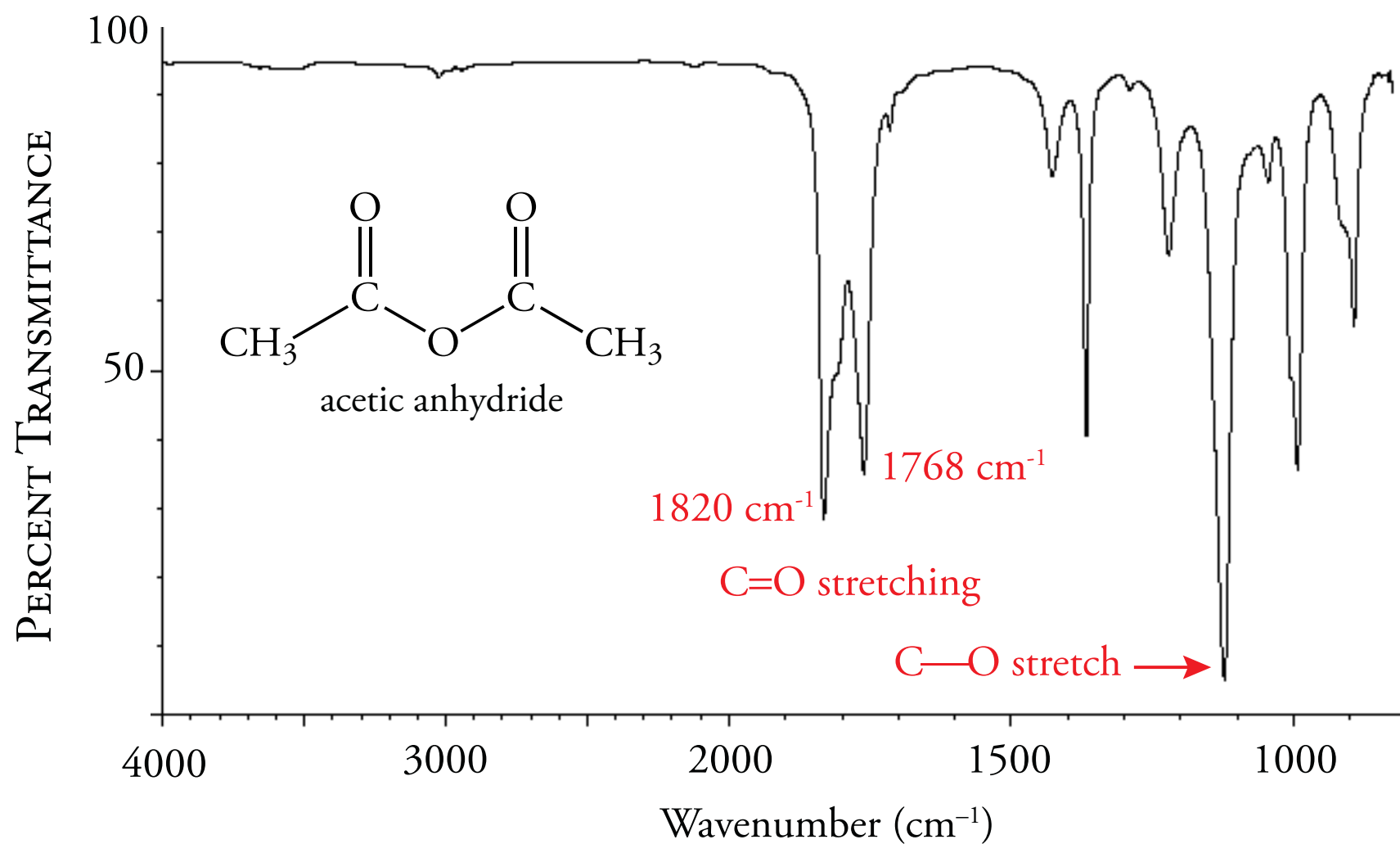
Figure 2.14 Infrared Spectrum of Ethyl Acetate



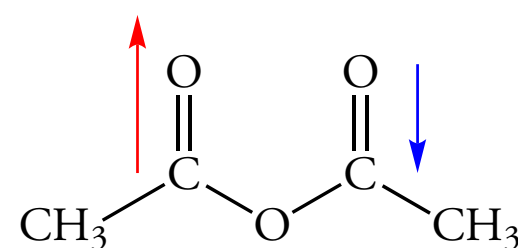
2.11 IDENTIFYING OXYGEN-CONTAINING COMPOUNDS

Carboxylic Acid Anhydrides

Figure 2.15 Infrared Spectrum of Acetic Anhydride



symmetric stretch
1820 cm^{-1}

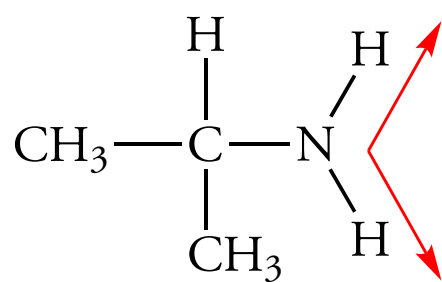
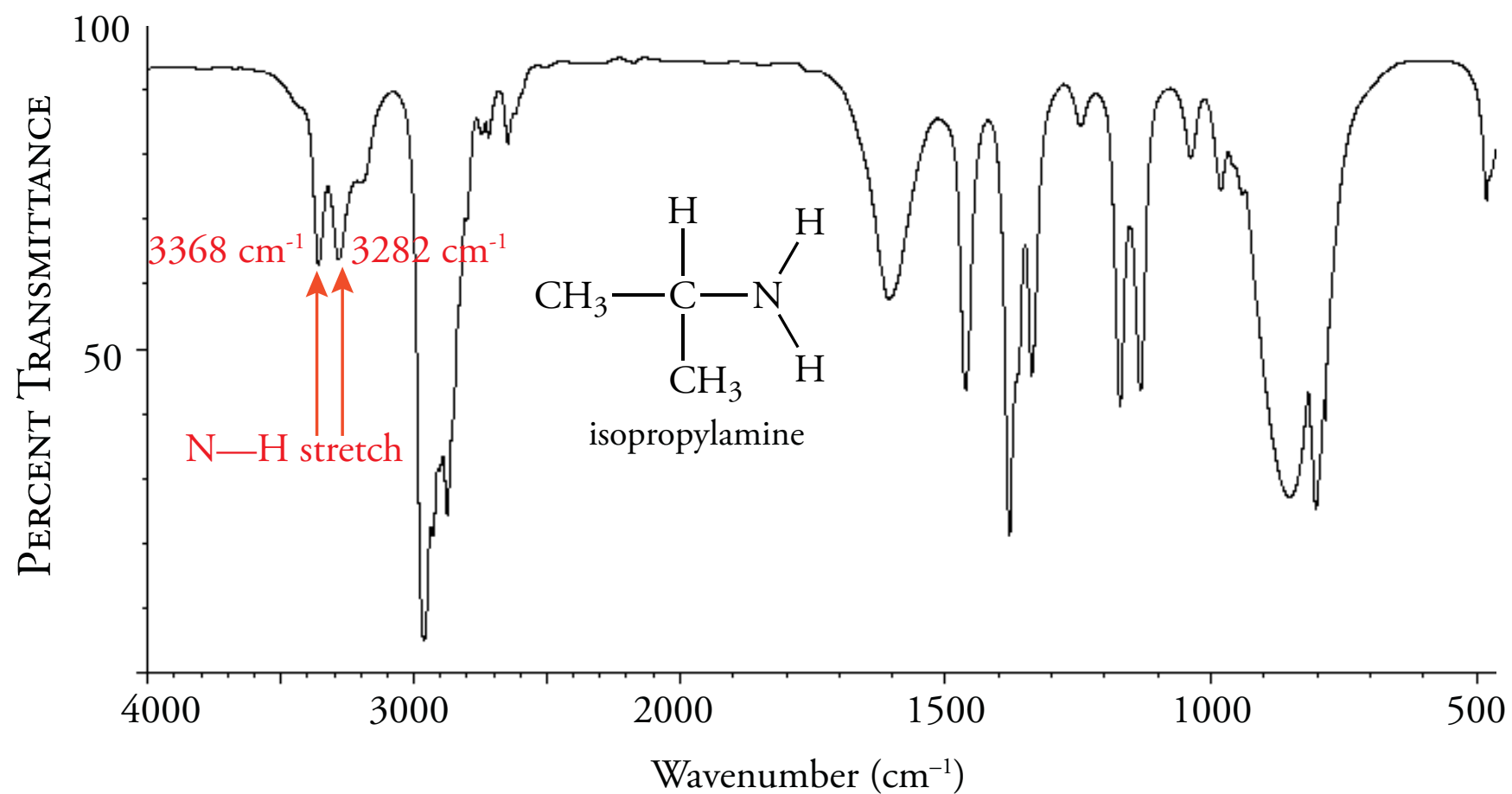


asymmetric stretch
1768 cm^{-1}

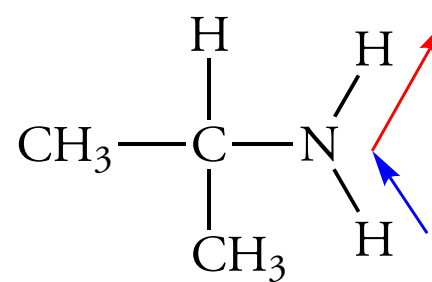
2.12 IDENTIFYING NITROGEN-CONTAINING COMPOUNDS

Amines

Figure 2.16 Infrared Spectrum of Isopropylamine



symmetric stretch
3368 cm^{-1}

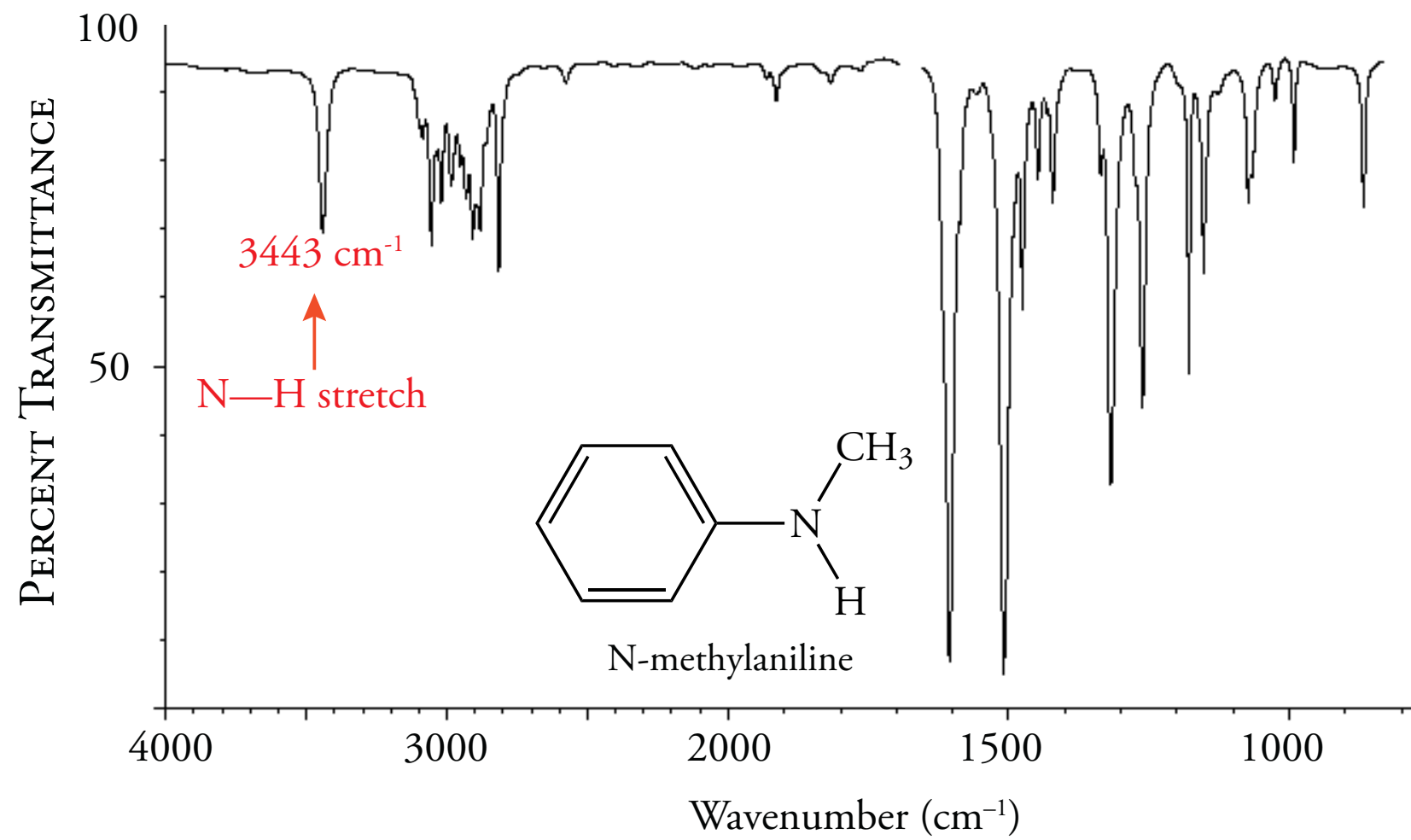


asymmetric stretch
3282 cm^{-1}

2.12 IDENTIFYING NITROGEN-CONTAINING COMPOUNDS

Amines

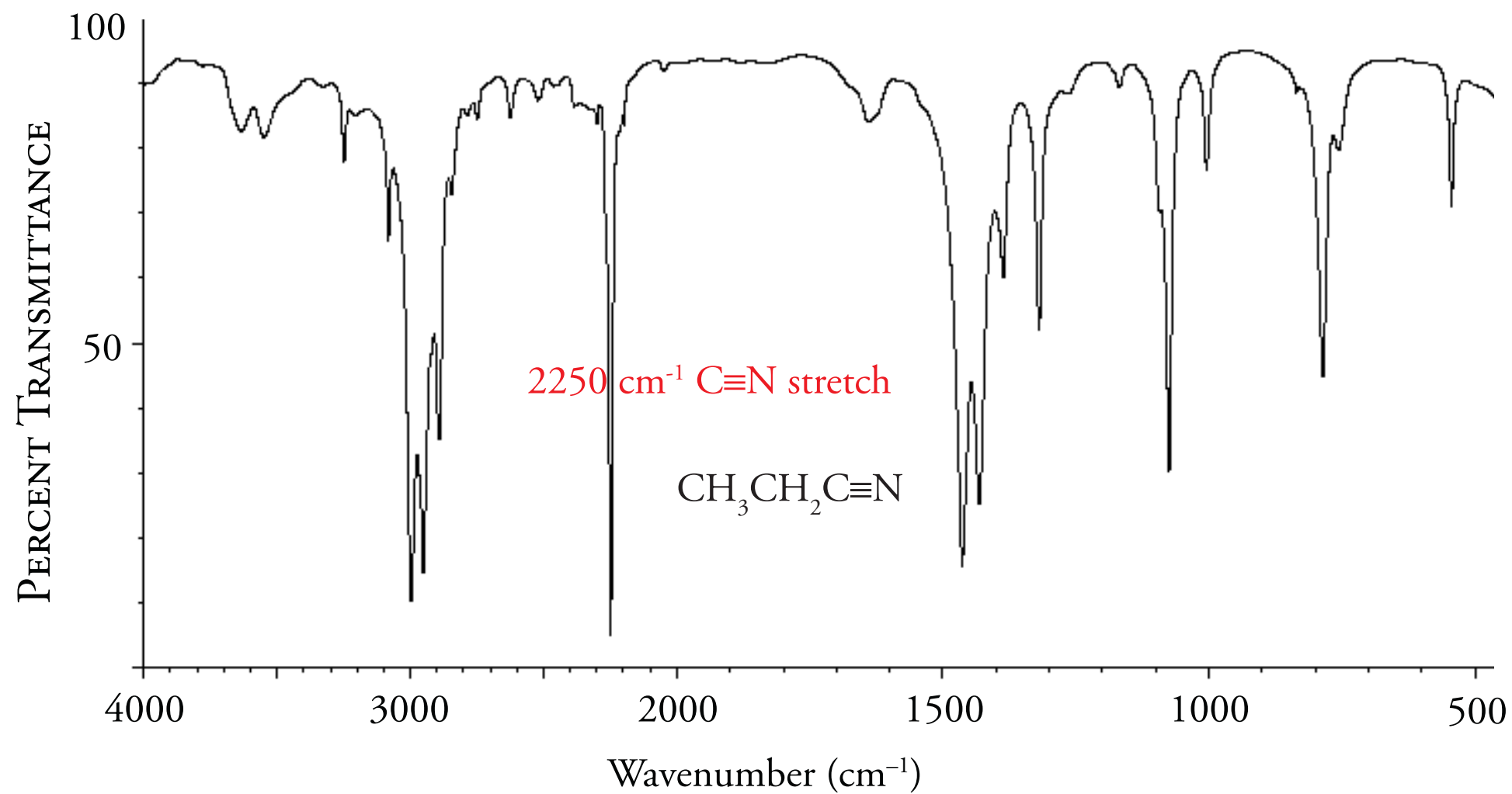
Figure 2.17 Infrared Spectrum of N-methylaniline



2.12 IDENTIFYING NITROGEN-CONTAINING COMPOUNDS

Nitriles

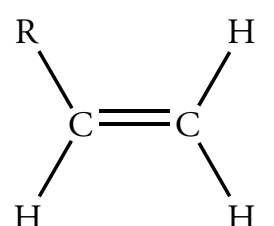
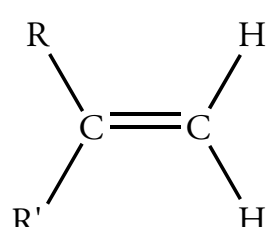
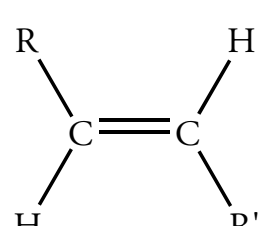
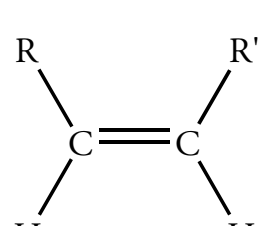
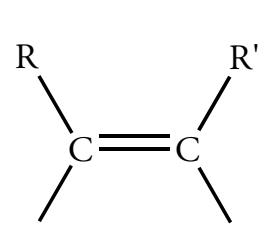
Figure 2.18 Infrared Spectrum of Propionitrile



2.13 BENDING DEFORMATIONS

Alkenes

Table 2.3
Out of Plane C—H Bending
Modes of Alkenes

<i>Bond</i>	<i>Absorption (cm⁻¹)</i>
	995-985 910-905
	895-885
	980-965
	690 (ambiguous)
	840-790

2.13 BENDING DEFORMATIONS

Bending Modes in Aromatic Compounds

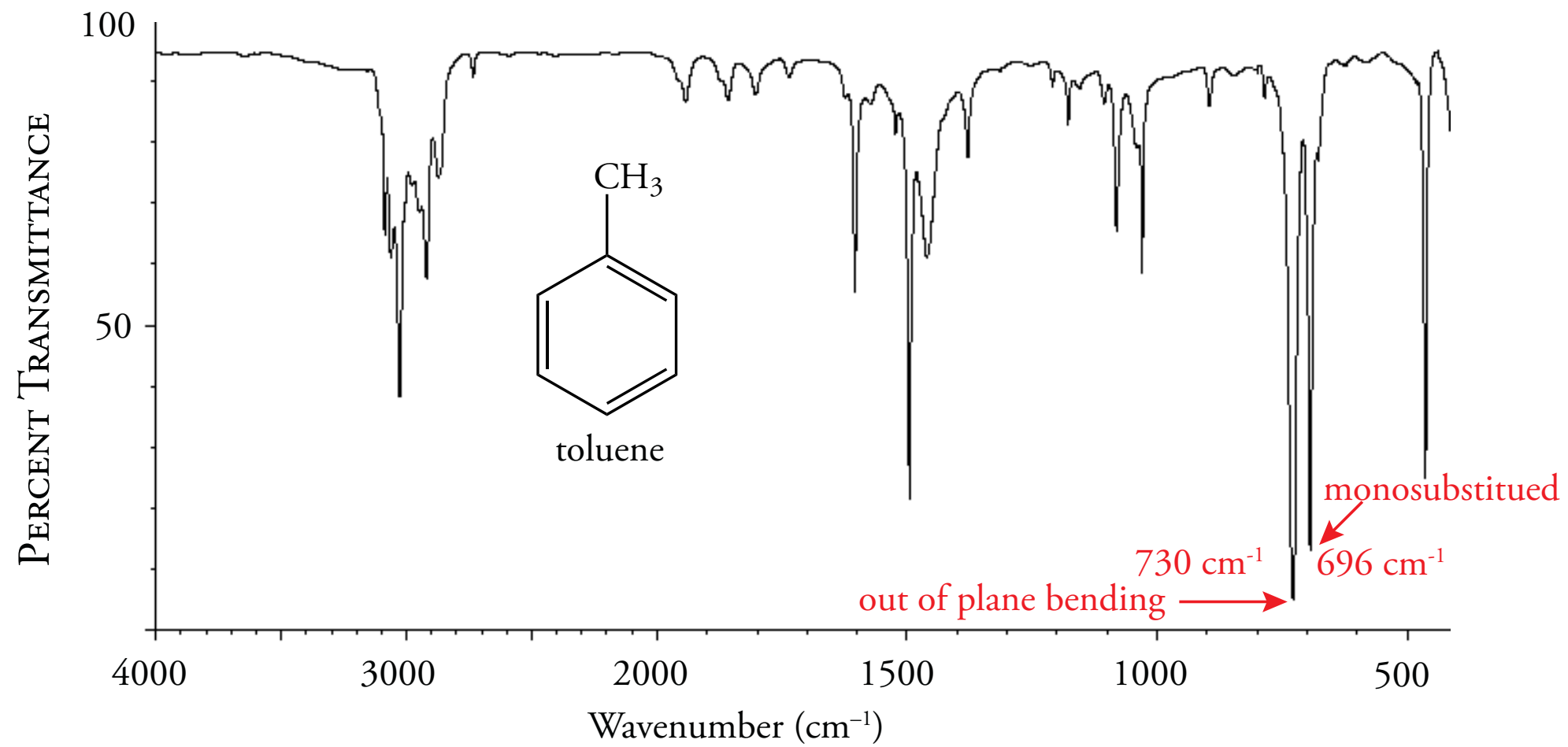
Table 2.4
Out of Plane Bending Modes of
Aromatic Ring Hydrogen Atoms

<i>Number of Adjacent Hydrogen Atoms</i>	<i>Wavenumber (cm^{-1})</i>
5	770-730
4	770-735
3	810-750
2	860-800
1	900-860

2.13 BENDING DEFORMATIONS

Bending Modes in Aromatic Compounds

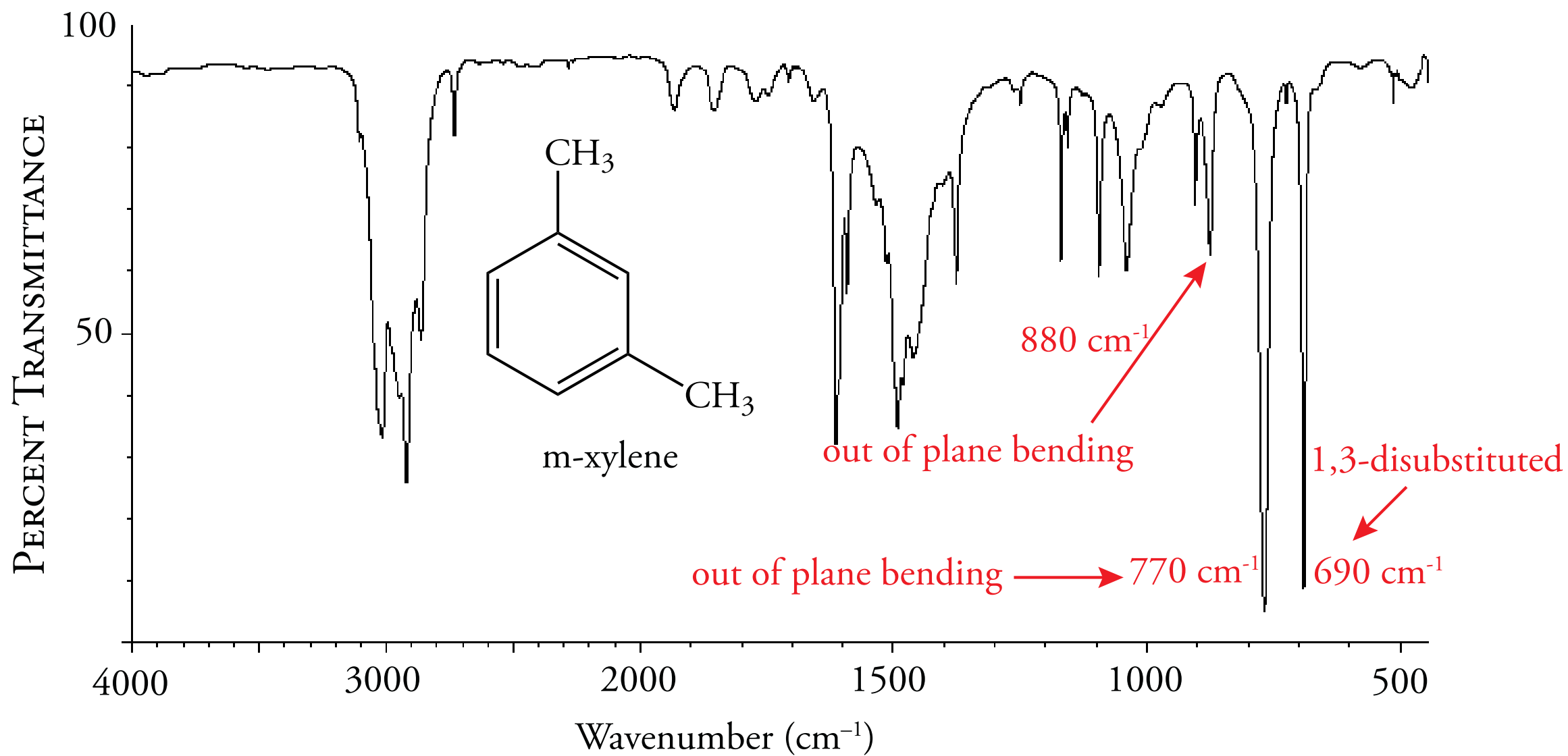
Figure 2.19 IR Spectrum of Toluene



2.13 BENDING DEFORMATIONS

Bending Modes in Aromatic Compounds

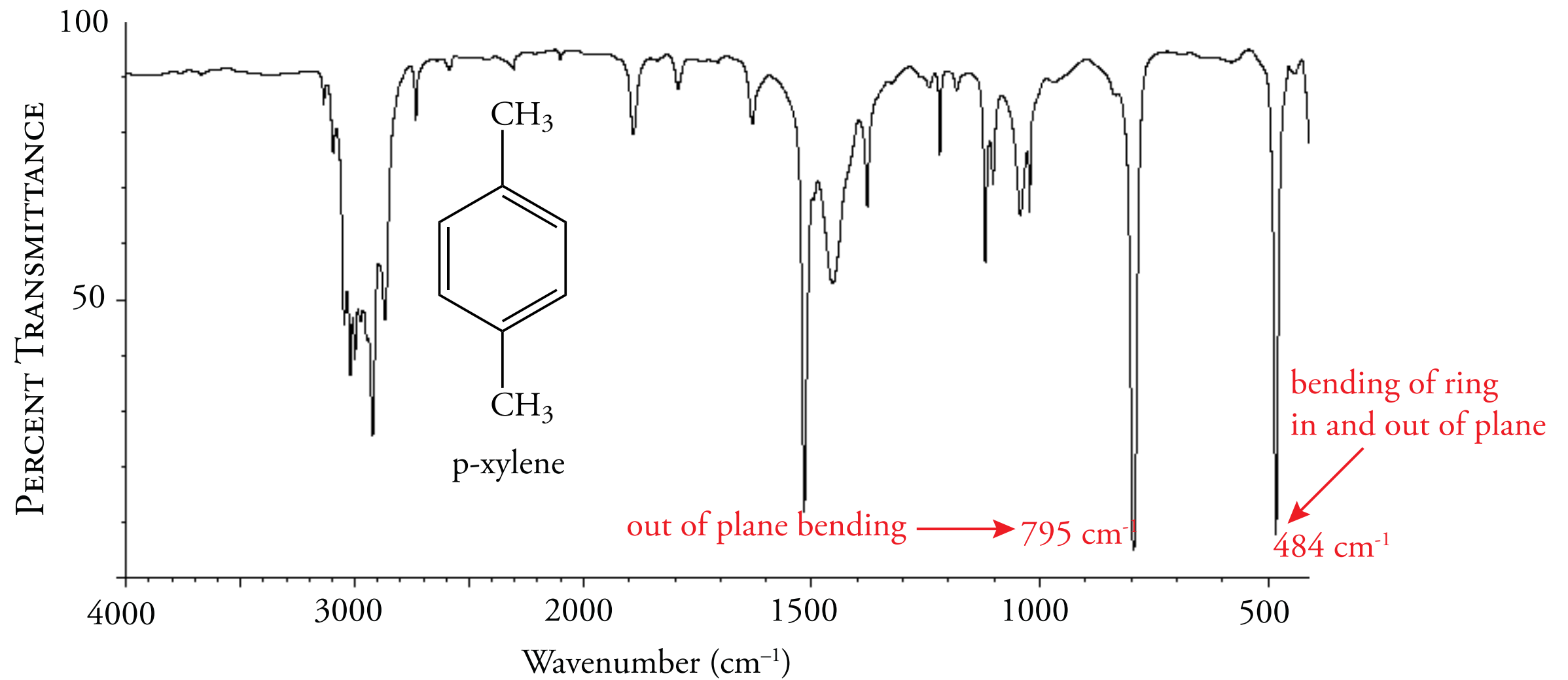
Figure 2.20 IR Spectrum of m-Xylene



2.13 BENDING DEFORMATIONS

Bending Modes in Aromatic Compounds

Figure 2.21 IR Spectrum of p-Xylene



2.13 BENDING DEFORMATIONS

Bending Modes in Aromatic Compounds

Figure 2.22 IR Spectrum of o-Xylene

