

Introduction to Infrared Spectroscopy

Gives information about the functional groups
in a molecule

Infrared Spectroscopy

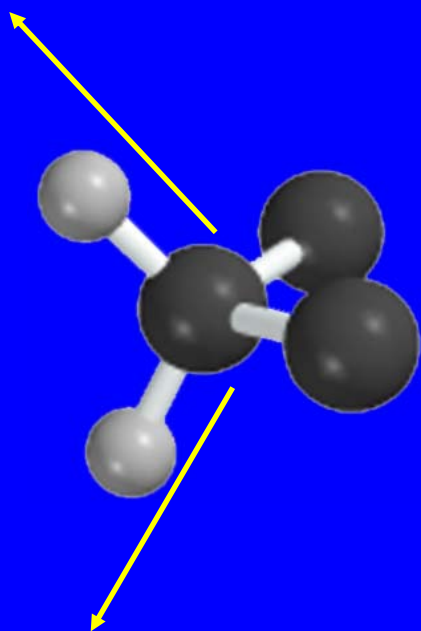
region of infrared that is most useful lies between
2.5-16 μm (4000-625 cm^{-1})

depends on transitions between vibrational
energy states

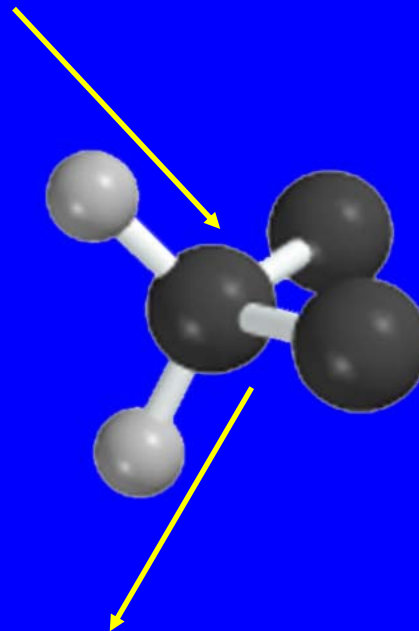
stretching

bending

Stretching Vibrations of a CH₂ Group

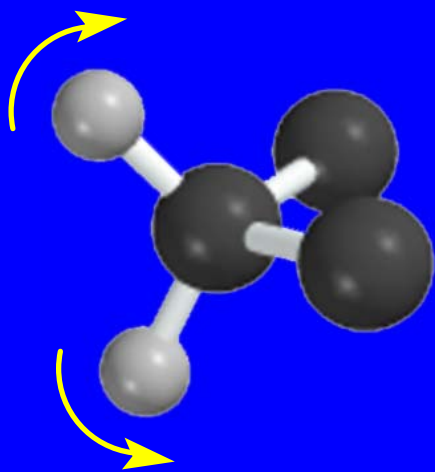


Symmetric

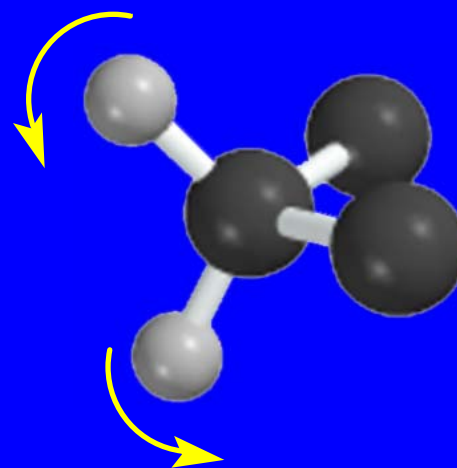


Antisymmetric

Bending Vibrations of a CH₂ Group

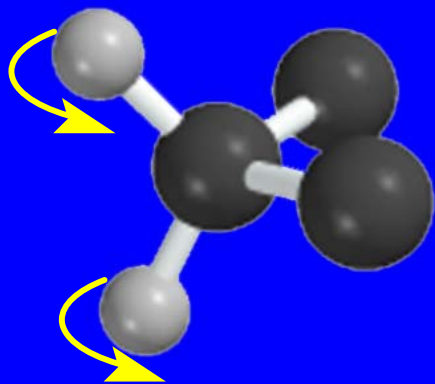


In plane

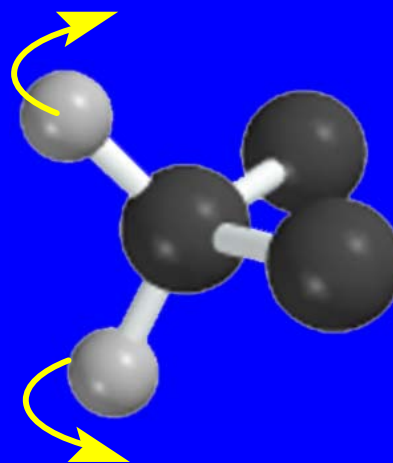


In plane

Bending Vibrations of a CH₂ Group



Out of plane



Out of plane

Infrared Spectroscopy

Infrared Spectroscopy

Characteristic functional groups usually found between 4000-1600 cm^{-1} .

From 1300-625 cm^{-1} called fingerprint region.

Insert Figure 13.30 here

Figure 13.31(a): Infrared Spectrum of Hexane

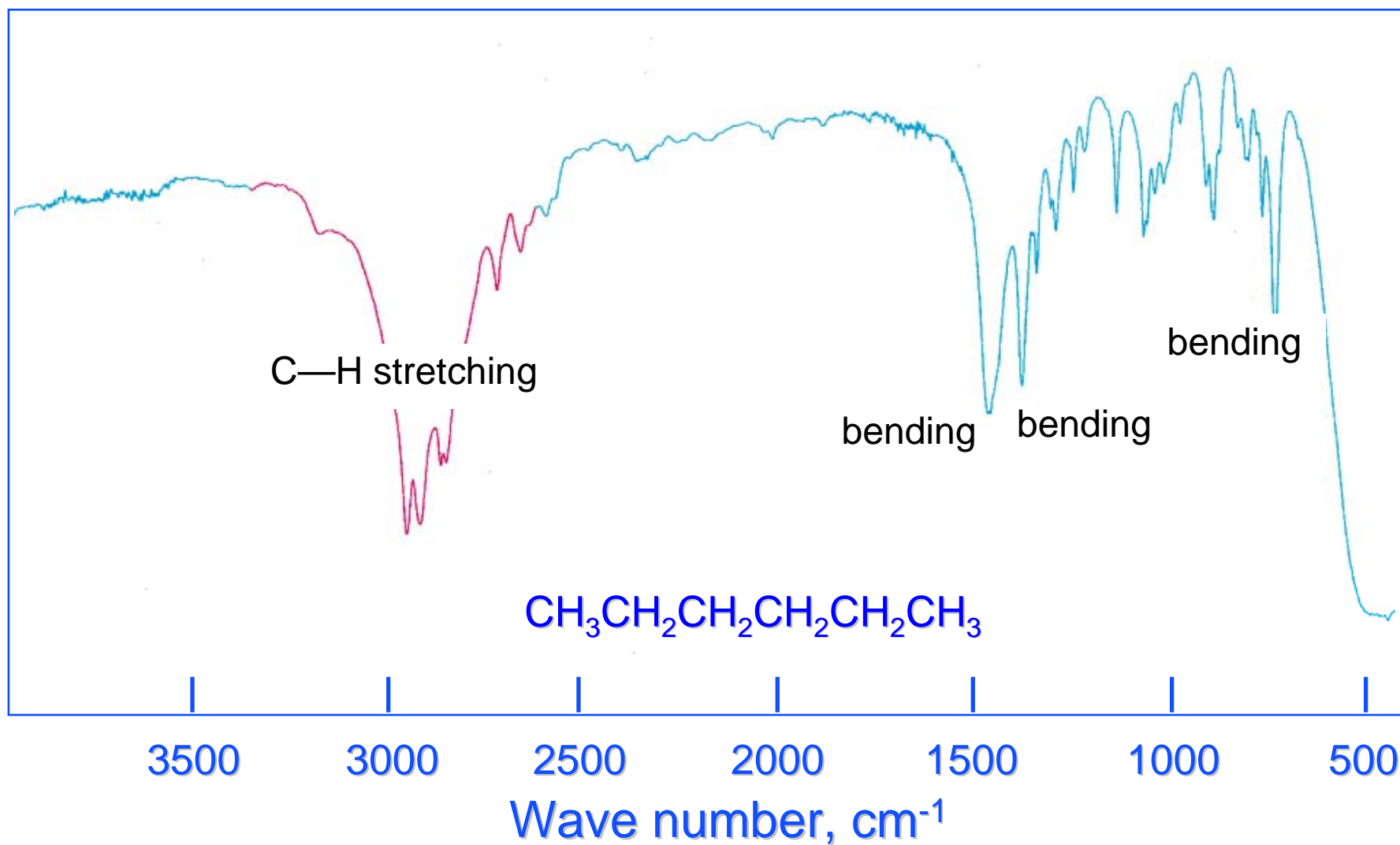
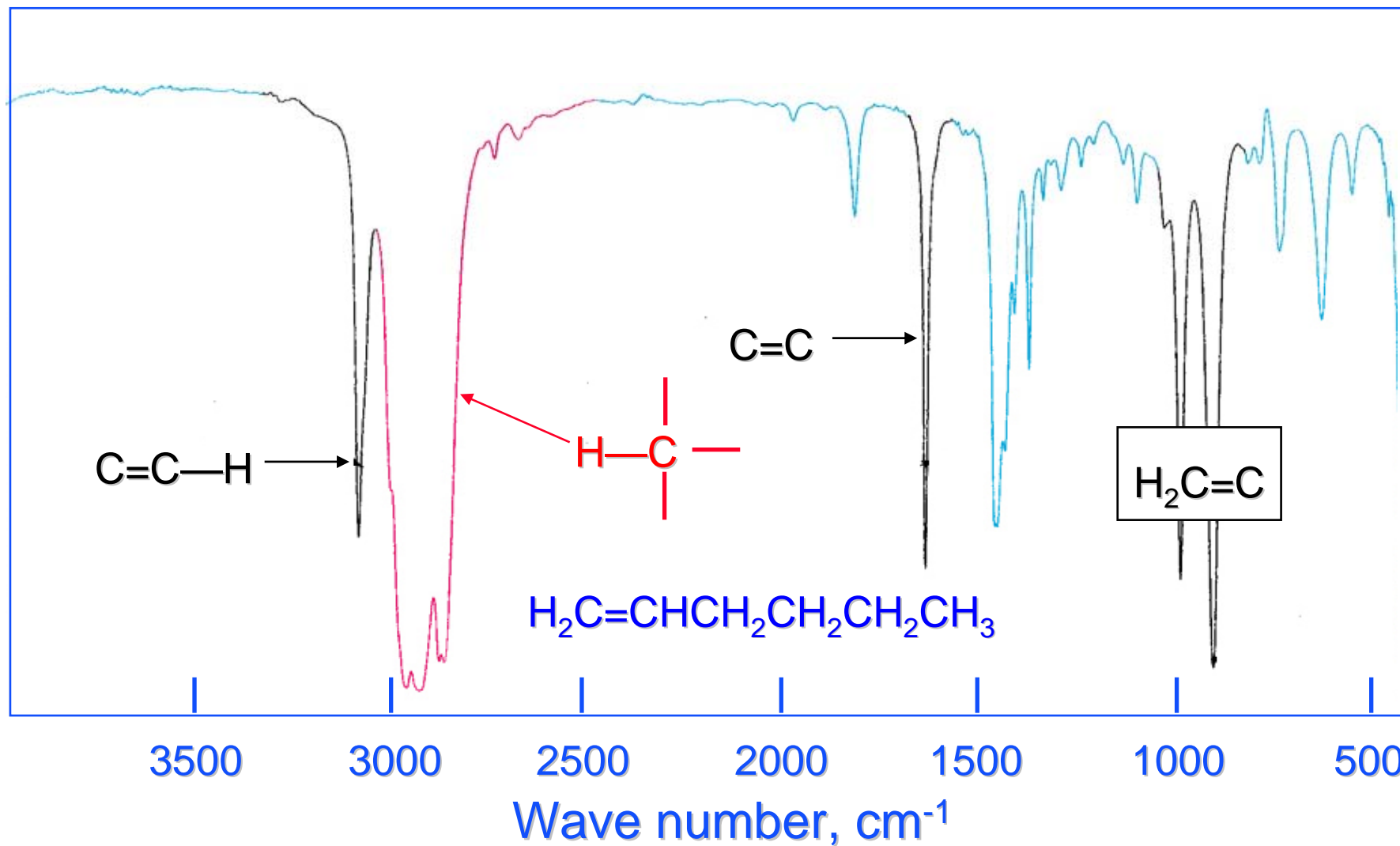


Figure 13.31(b): Infrared Spectrum of 1-Hexene



Characteristic Absorption Frequencies

Table 13.4
Infrared Absorption Frequencies

Structural unit	Frequency, cm^{-1}
Stretching vibrations (single bonds)	
sp C—H	3310-3320
sp^2 C—H	3000-3100
sp^3 C—H	2850-2950
sp^2 C—O	1200
sp^3 C—O	1025-1200

Figure 13.32(f): Infrared Spectrum of Diethyl Ether

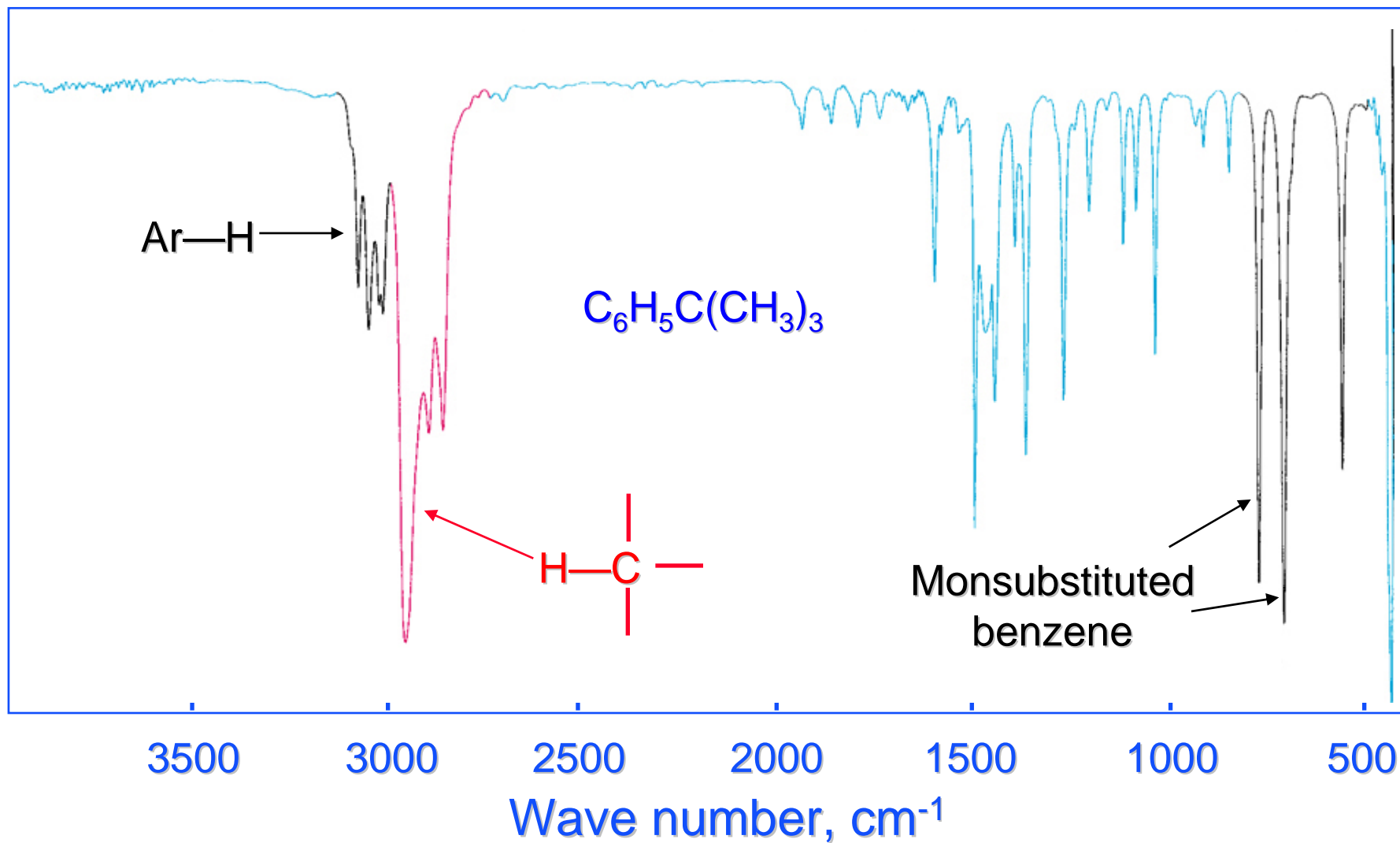
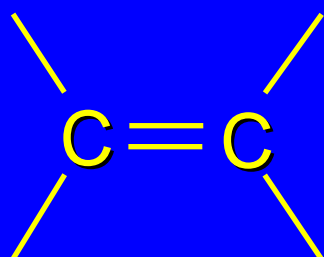


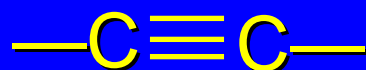
Table 13.4
Infrared Absorption Frequencies

Structural unit Frequency, cm^{-1}

Stretching vibrations (multiple bonds)



1620-1680



2100-2200



2240-2280

Figure 13.32(b): Infrared Spectrum of Hexanenitrile

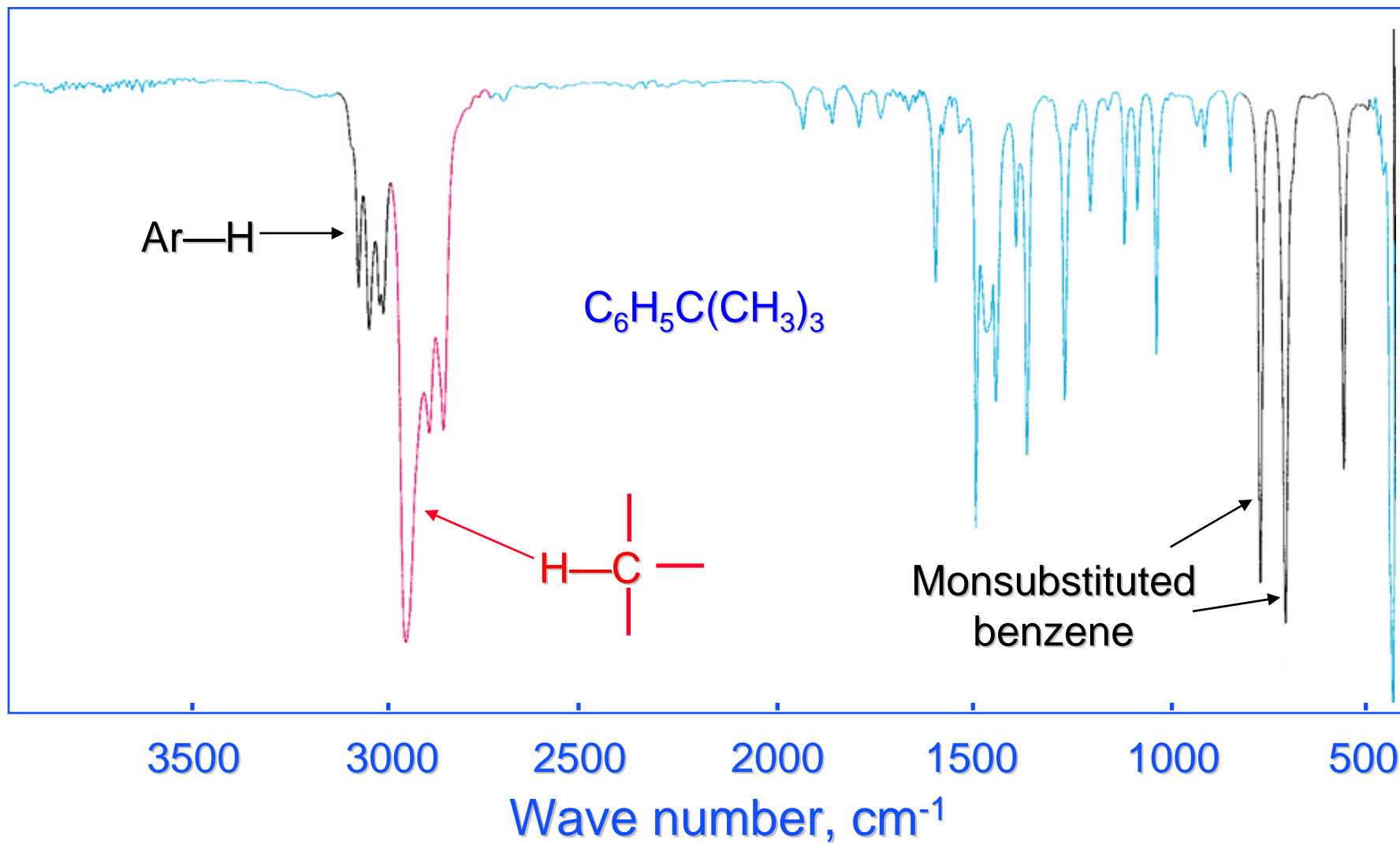


Table 13.4
Infrared Absorption Frequencies

Structural unit	Frequency, cm^{-1}
Stretching vibrations (carbonyl groups)	
Aldehydes and ketones	1710-1750
Carboxylic acids	1700-1725
Acid anhydrides	1800-1850 and 1740-1790
Esters	1730-1750
Amides	1680-1700

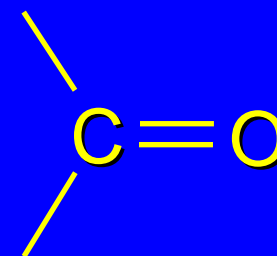


Figure 13.32(d): Infrared Spectrum of 2-Hexanone

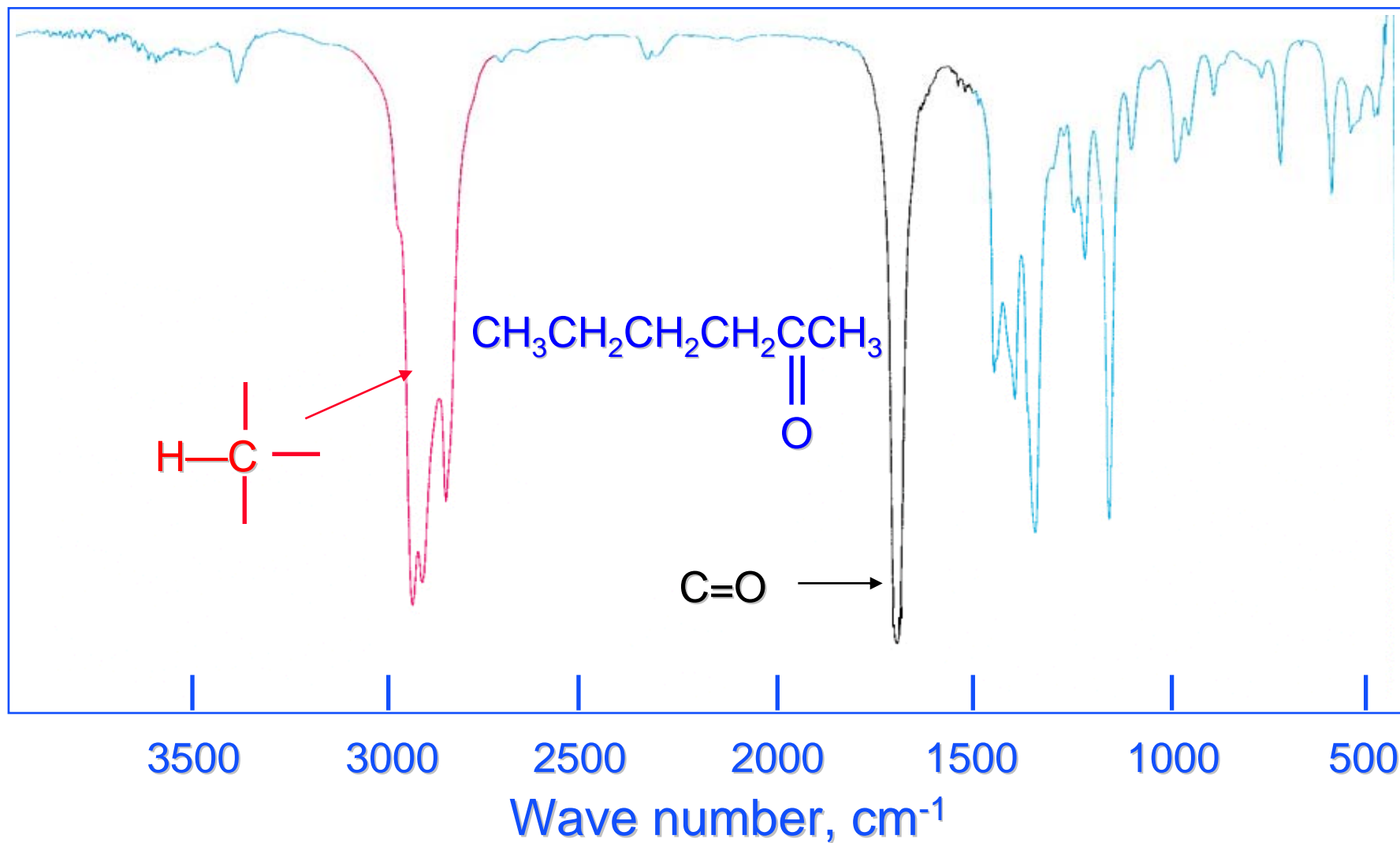


Figure 13.32(e): Infrared Spectrum of Methyl Hexanoate

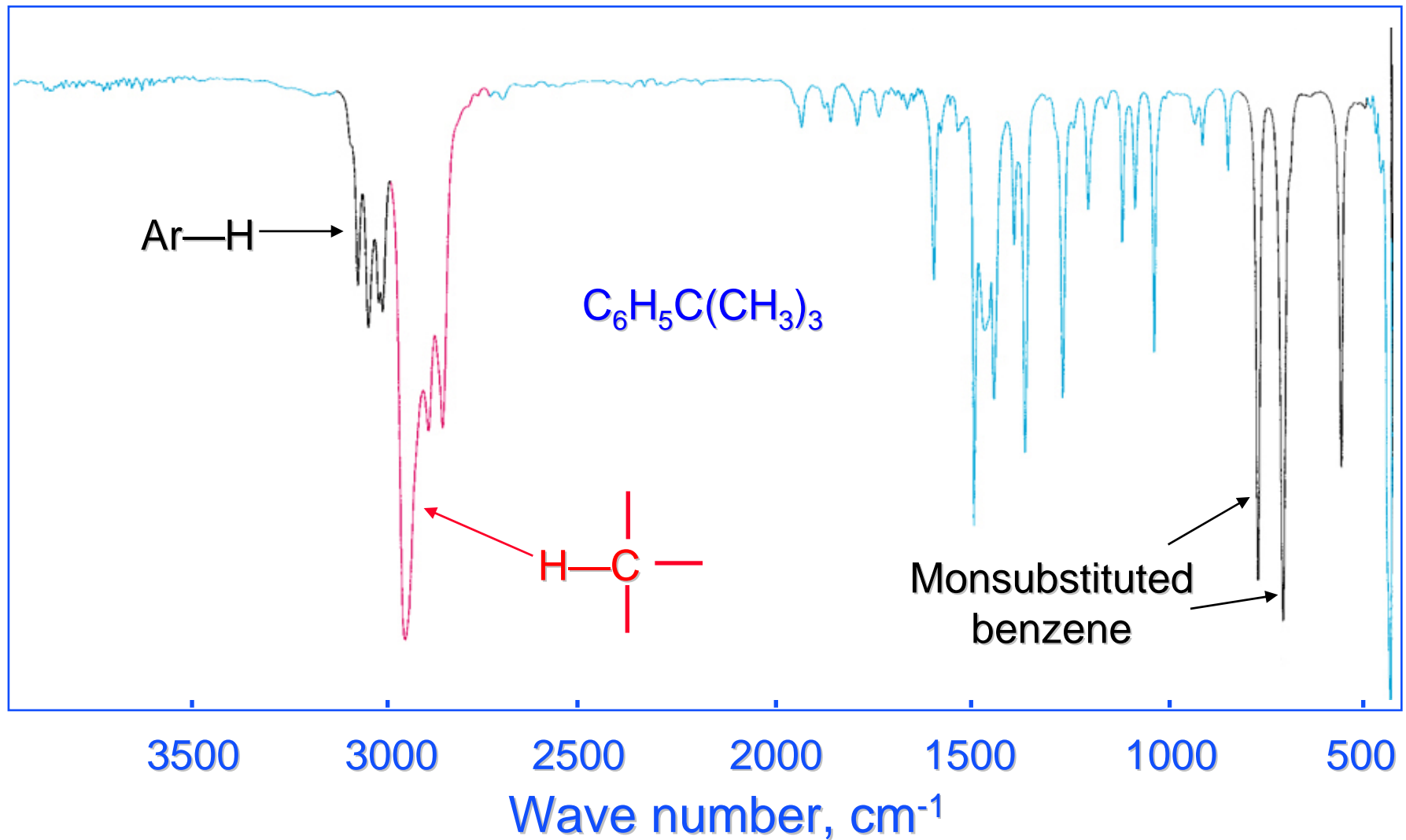


Table 13.4
Infrared Absorption Frequencies

Structural unit	Frequency, cm^{-1}
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Bending vibrations of alkenes

$\text{RCH}=\text{CH}_2$	910-990
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$\text{R}_2\text{C}=\text{CH}_2$	890
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<i>cis</i> - $\text{RCH}=\text{CHR}'$	665-730
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<i>trans</i> - $\text{RCH}=\text{CHR}'$	960-980
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$\text{R}_2\text{C}=\text{CHR}'$	790-840
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Table 13.4
Infrared Absorption Frequencies

Structural unit	Frequency, cm^{-1}
Bending vibrations of derivatives of benzene	
Monosubstituted	730-770 and 690-710
Ortho-disubstituted	735-770
Meta-disubstituted	750-810 and 680-730
Para-disubstituted	790-840

Table 13.4
Infrared Absorption Frequencies

Structural unit	Frequency, cm^{-1}
Stretching vibrations (single bonds)	
O—H (alcohols)	3200-3600
O—H (carboxylic acids)	3000-3100
N—H	3350-3500

Figure 13.32(a): Infrared Spectrum of 1-Hexanol

