13.19

Infrared Spectroscopy

Gives information about the functional groups in a molecule

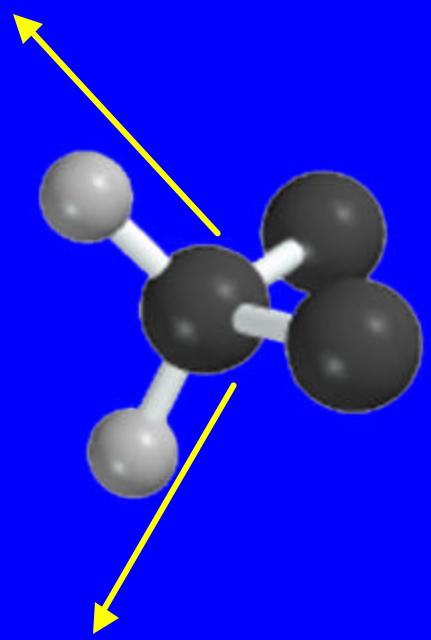
Infrared Spectroscopy

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

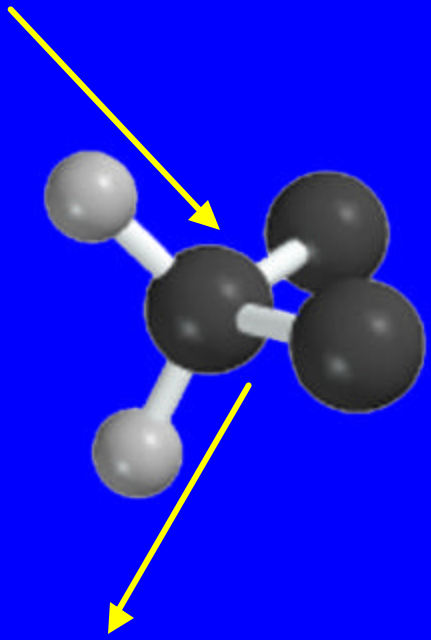
depends on transitions between vibrational energy states

- stretching
- bending

Stretching Vibrations of a CH_2 Group

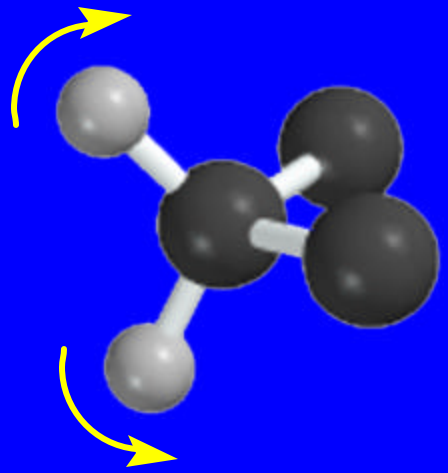


Symmetric

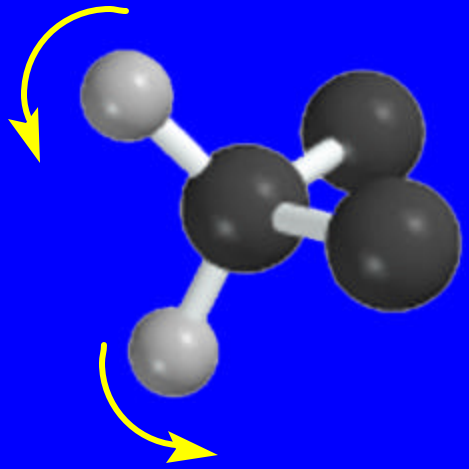


Antisymmetric

Bending Vibrations of a CH_2 Group

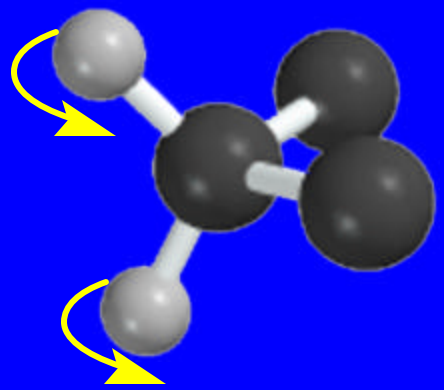


In plane

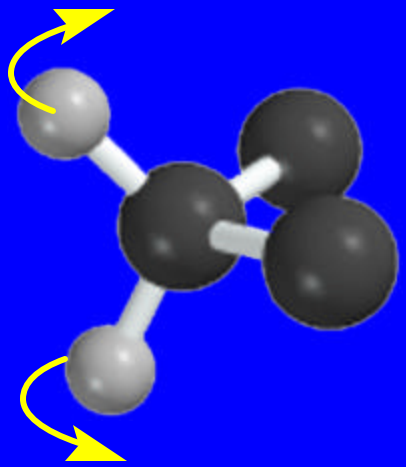


In plane

Bending Vibrations of a CH_2 Group



Out of plane



Out of plane

Figure 13.26: Infrared Spectrum of Hexane

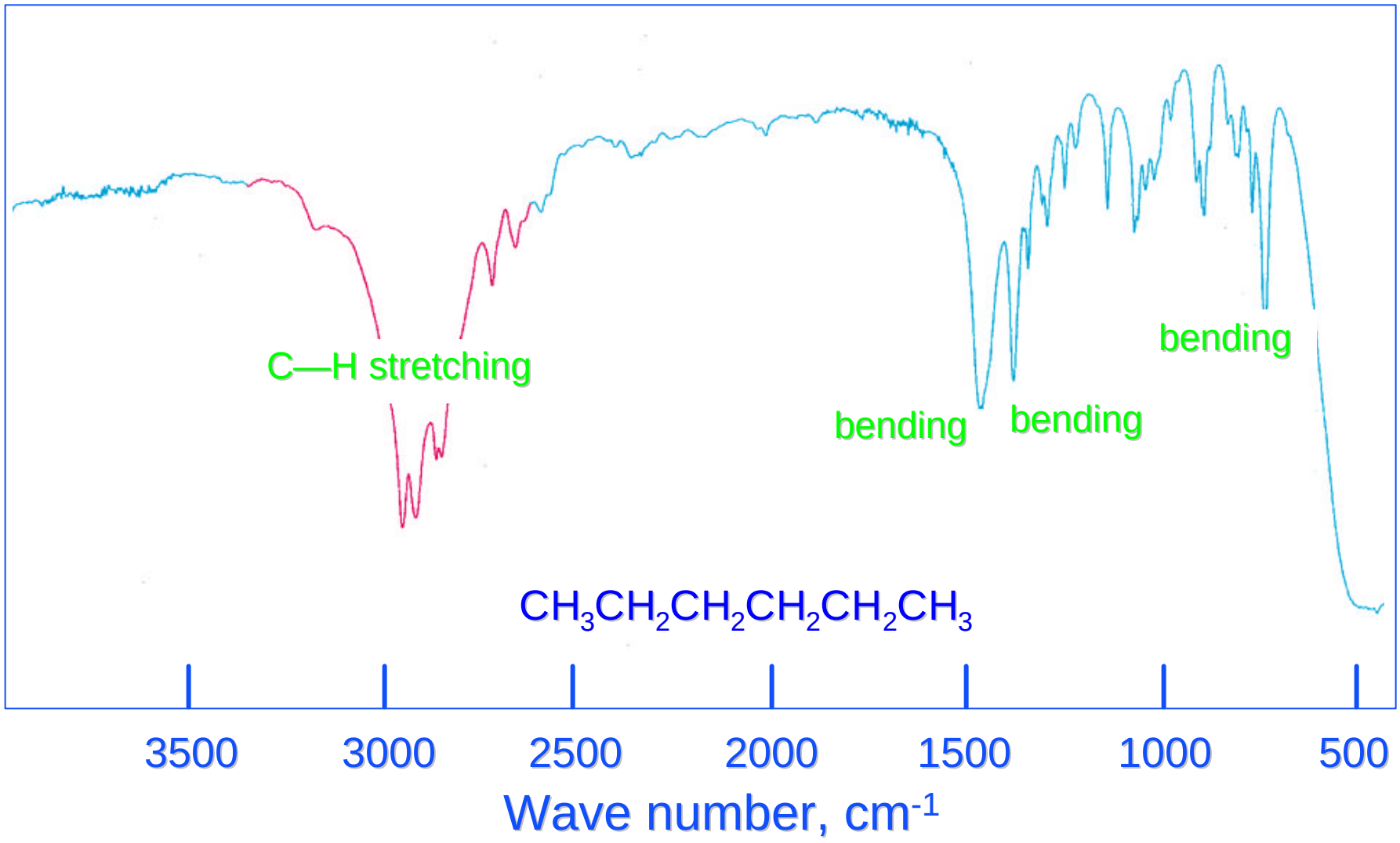


Figure 13.27: Infrared Spectrum of 1-Hexene

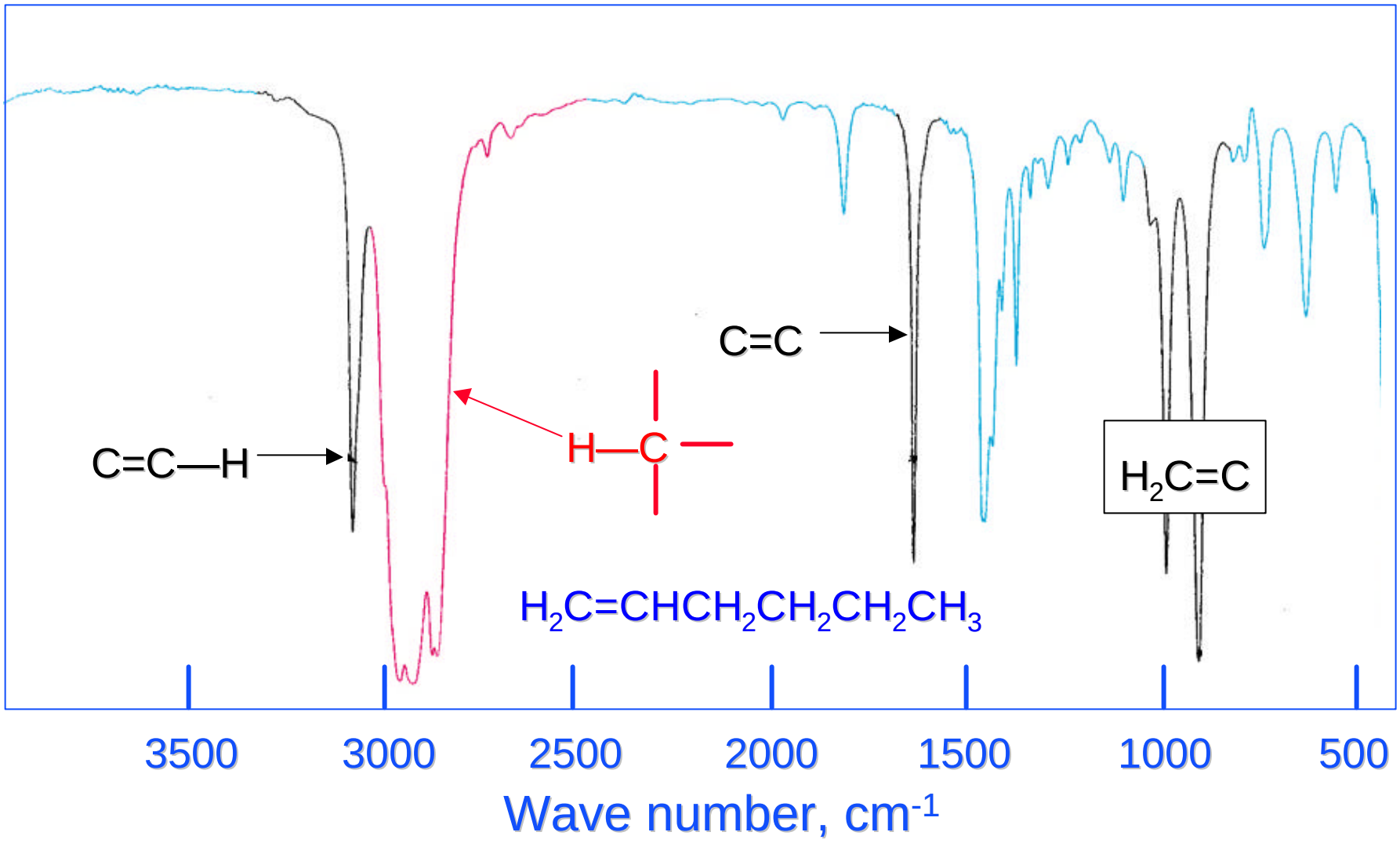


Table 13.4 (p 519)
Infrared Absorption Frequencies

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

Table 13.4 (p 519)
Infrared Absorption Frequencies

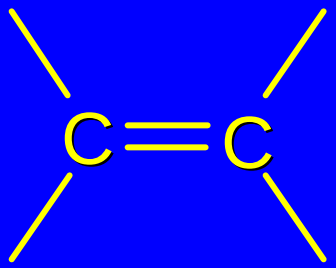
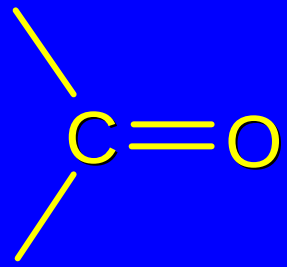
Structural unit	Frequency, cm^{-1}
Stretching vibrations (multiple bonds)	
	1620-1680
—C≡C—	2100-2200
—C≡N	2240-2280

Table 13.4 (p 519)
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

Table 13.4 (p 519)
Infrared Absorption Frequencies

Structural unit	Frequency, cm^{-1}
Bending vibrations of alkenes	
$RCH{=}CH_2$	910-990
$R_2C{=}CH_2$	890
cis-$RCH{=}CHR'$	665-730
trans-$RCH{=}CHR'$	960-980
$R_2C{=}CHR'$	790-840

Table 13.4 (p 519)
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

Figure 13.28: Infrared Spectrum of tert-*butylbenzene*

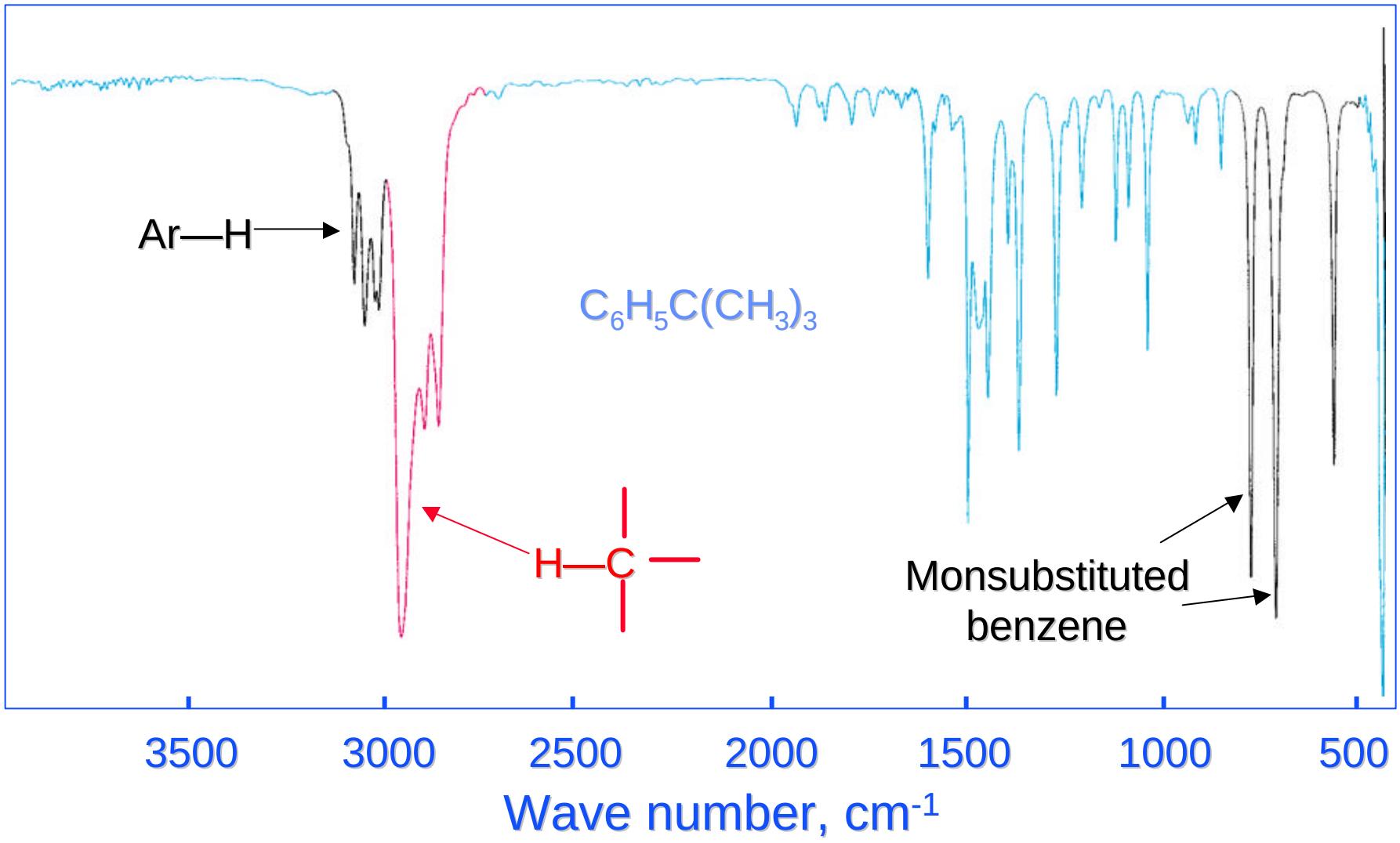


Table 13.4 (p 519)
Infrared Absorption Frequencies

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 13.29: Infrared Spectrum of 2-Hexanol

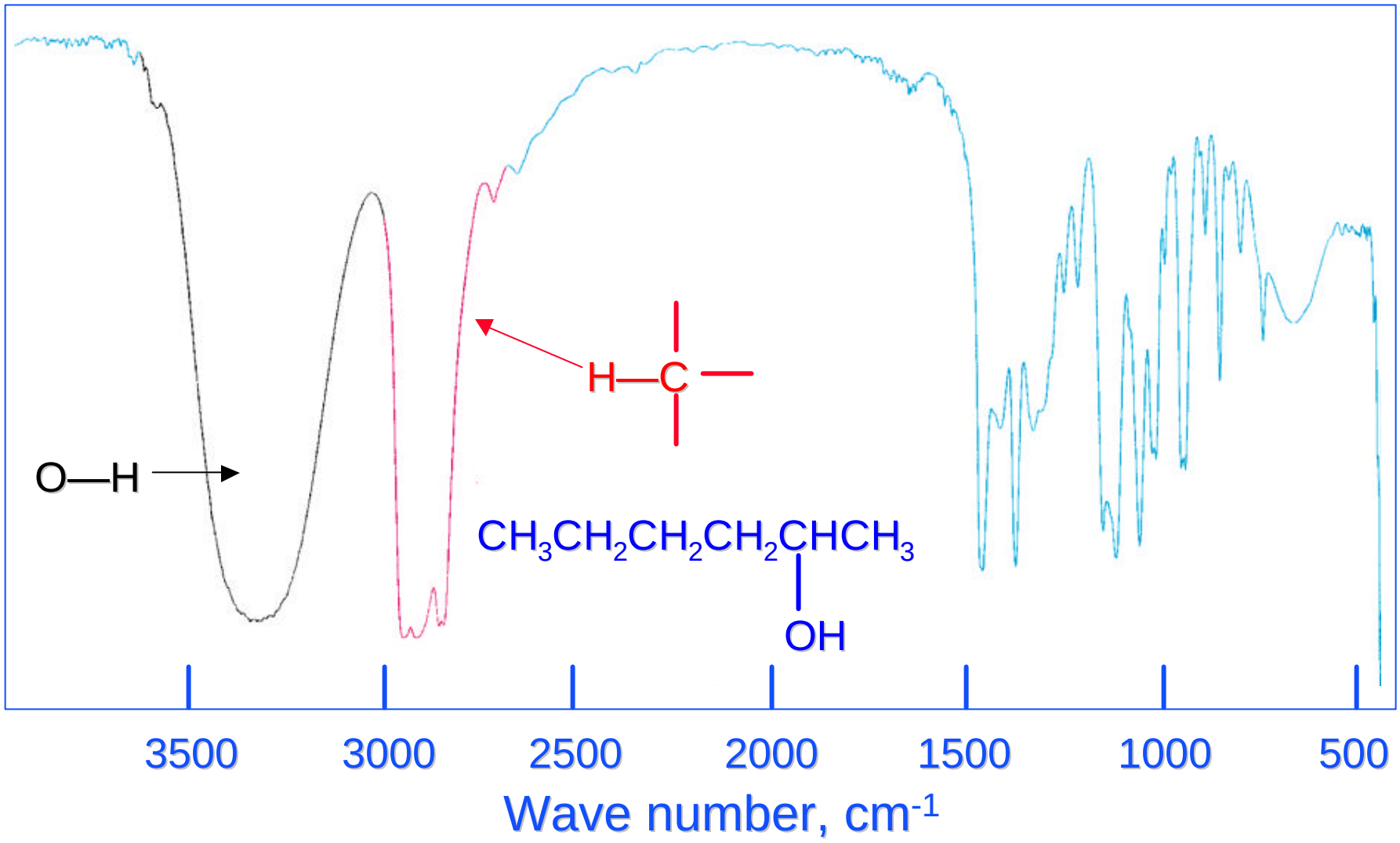


Figure 13.29: Infrared Spectrum of 2-Hexanone