Section 19.18
Spectroscopic Analysis of Carboxylic Acids

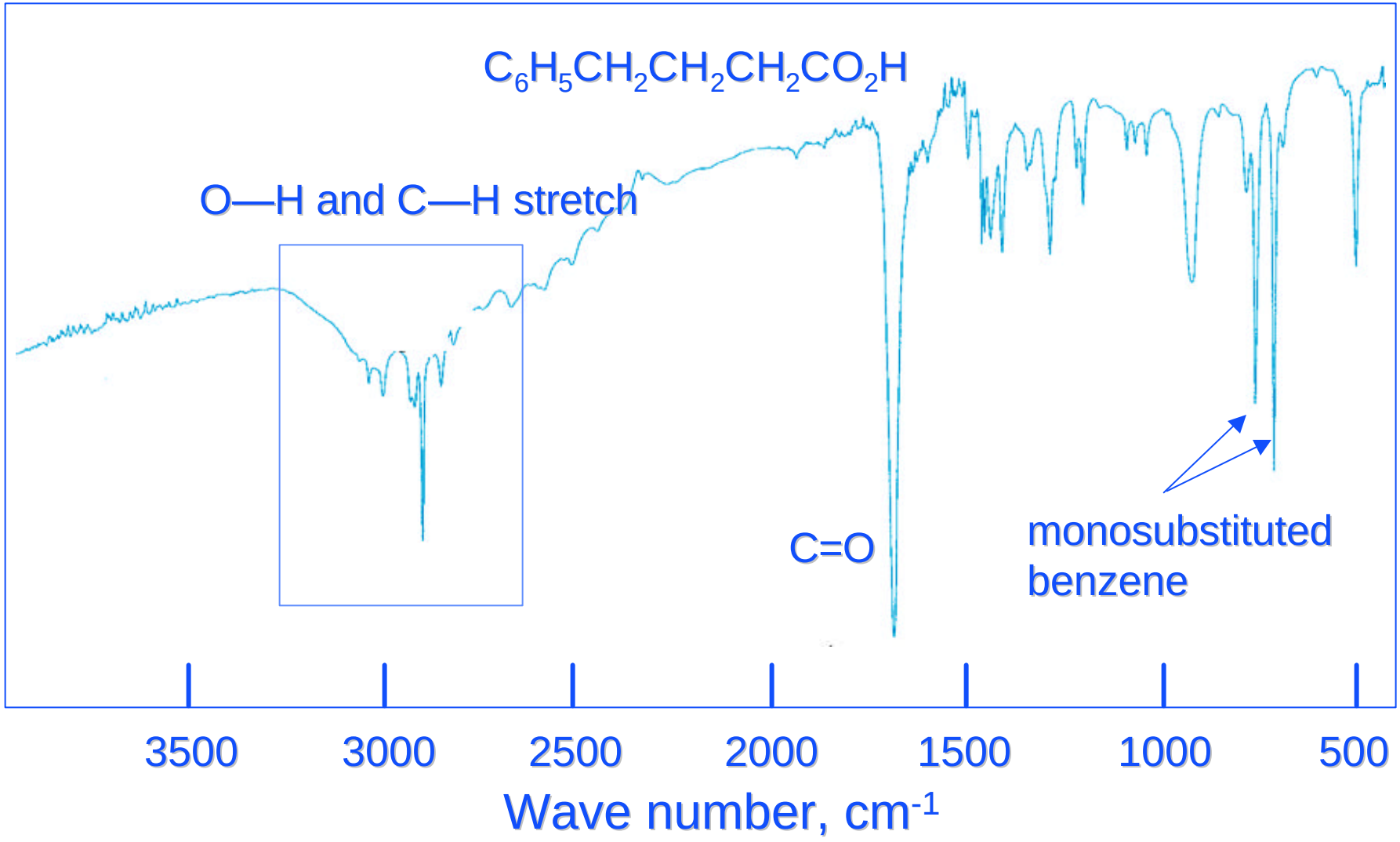
Infrared Spectroscopy

A carboxylic acid is characterized by peaks due to OH and C=O groups in its infrared spectrum.

C=O stretching gives an intense absorption near 1700 cm^{-1}.

OH peak is broad and overlaps with C—H absorptions.

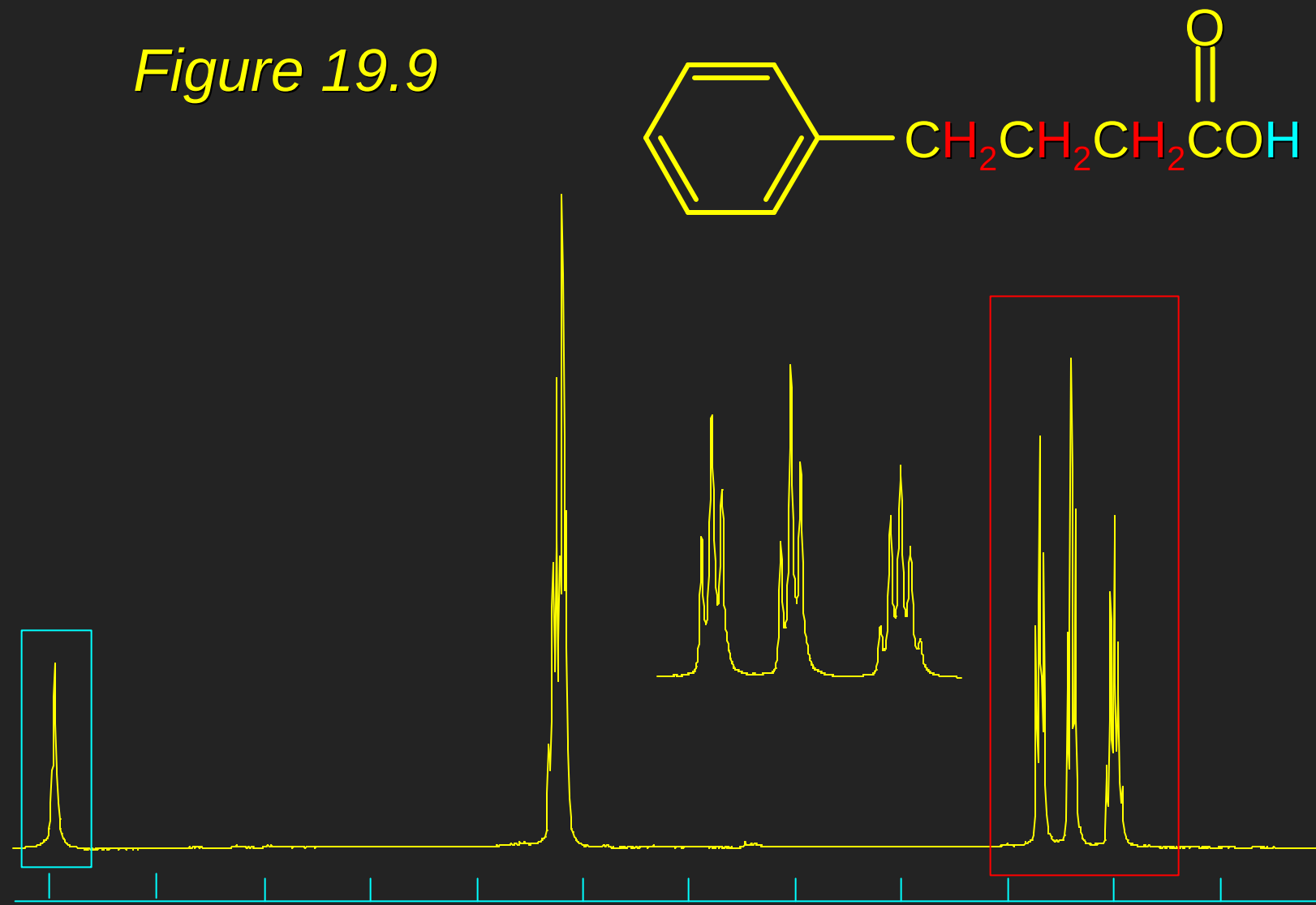
Figure 19.8 Infrared Spectrum of 4-Phenylbutanoic acid



^{1}H NMR

proton of OH group of a carboxylic acid is normally the least shielded of all of the protons in a ^{1}H NMR spectrum: (δ 10-12 ppm; broad).

Figure 19.9


CH2CH2CH2COH
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
Chemical shift (δ, ppm)

^{13}C NMR

Carbonyl carbon is at low field (δ 160-185 ppm), but not as deshielded as the carbonyl carbon of an aldehyde or ketone (δ 190-215 ppm).

UV-VIS

Carboxylic acids absorb near 210 nm, but UV-VIS spectroscopy has not proven to be very useful for structure determination of carboxylic acids.

Mass Spectrometry

Aliphatic carboxylic acids undergo a variety of fragmentations.

Aromatic carboxylic acids first form acylium ions, which then lose CO.