Section 17.17
Spectroscopic Analysis of Aldehydes and Ketones

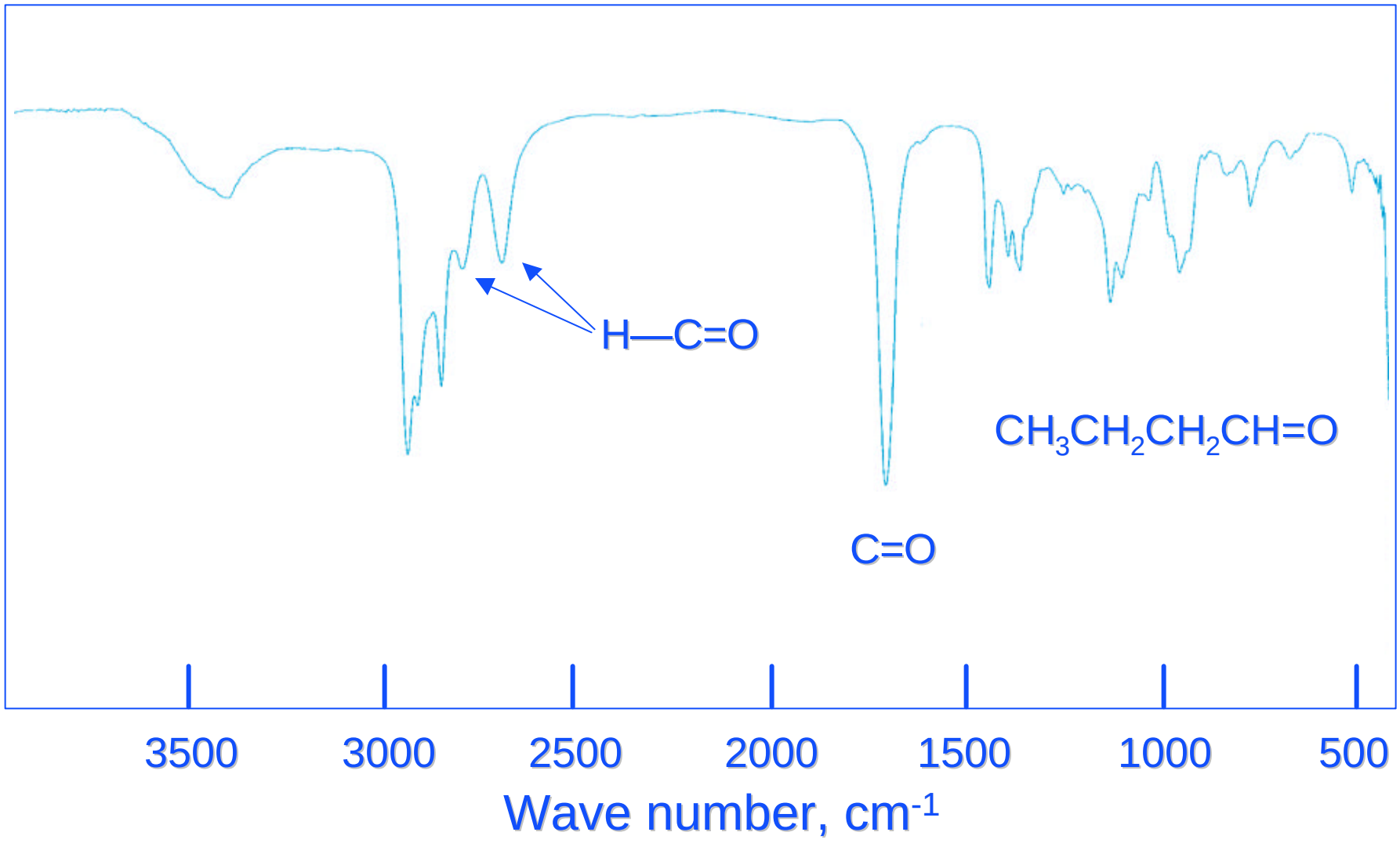
Infrared Spectroscopy

Presence of a C=O group is readily apparent in infrared spectrum

C=O stretching gives an intense absorption at 1710-1750 cm-1

In addition to peak for C=O, aldehydes give two weak peaks near 2720 and 2820 nm for H—C=O

Figure 17.13 Infrared Spectrum of Butanal



^{1}H NMR

Aldehydes: H—C=O proton is at very low field (δ 9-10 ppm).

Methyl ketones: CH_3 singlet near δ 2 ppm.

Figure 17.14

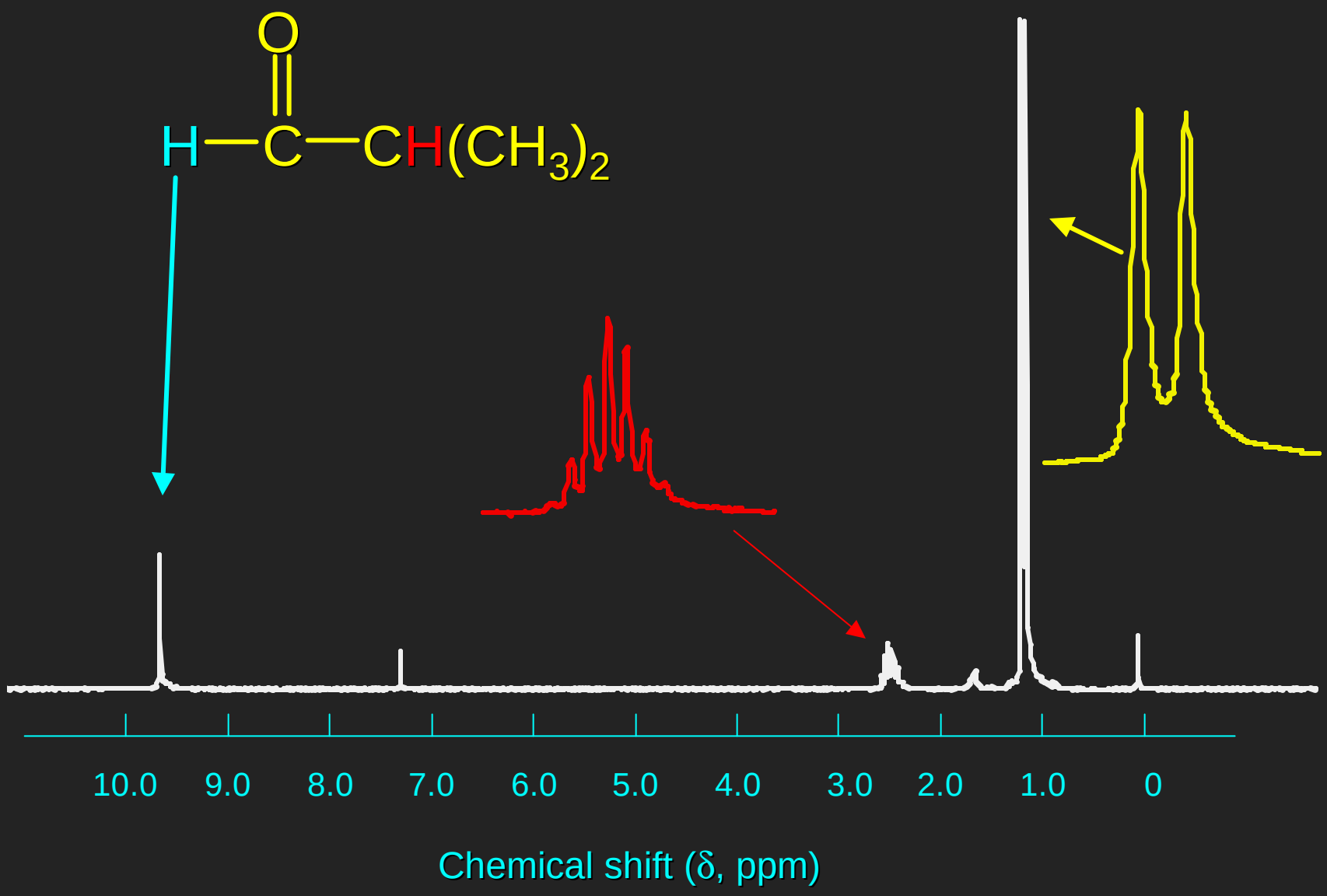
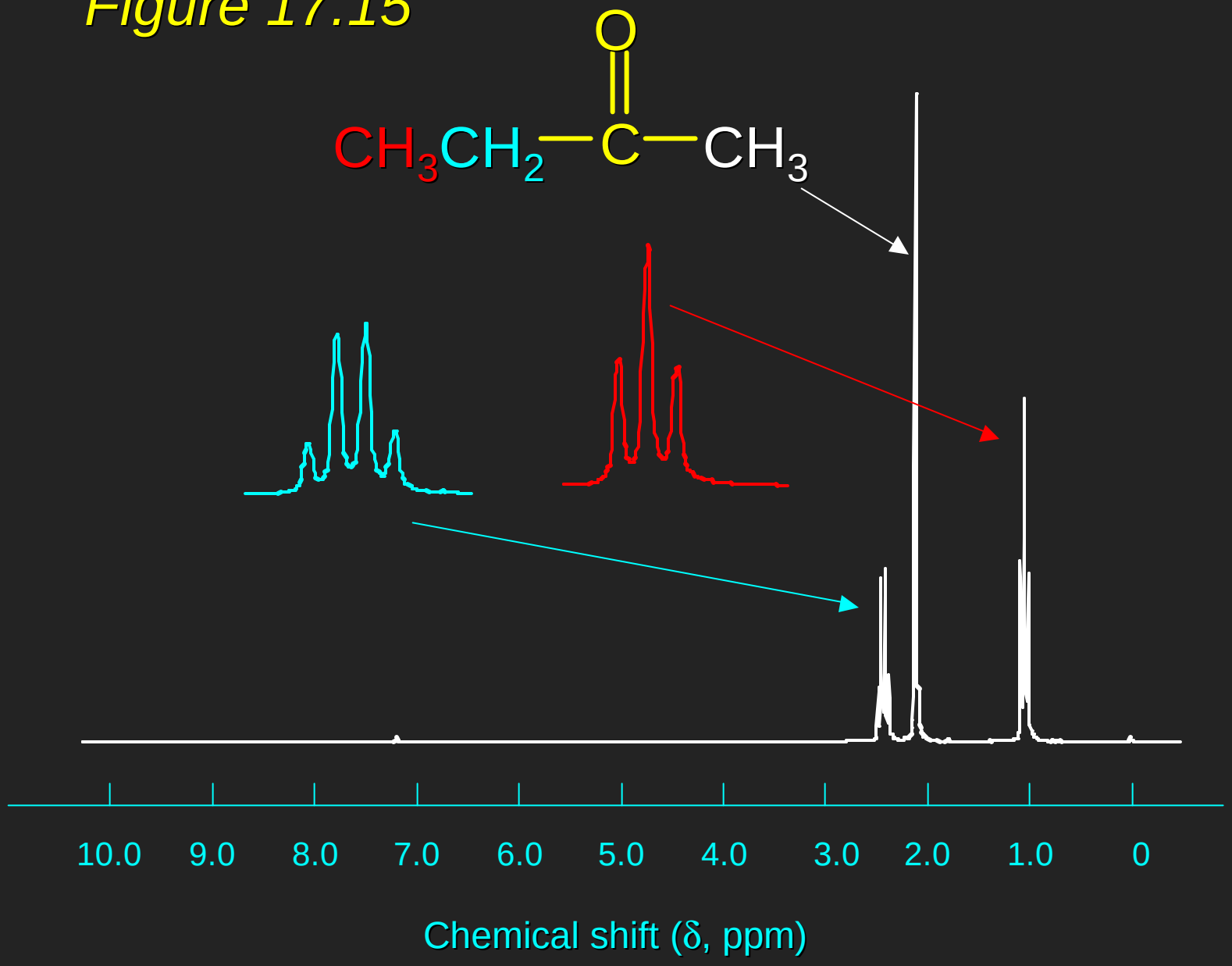


Figure 17.15

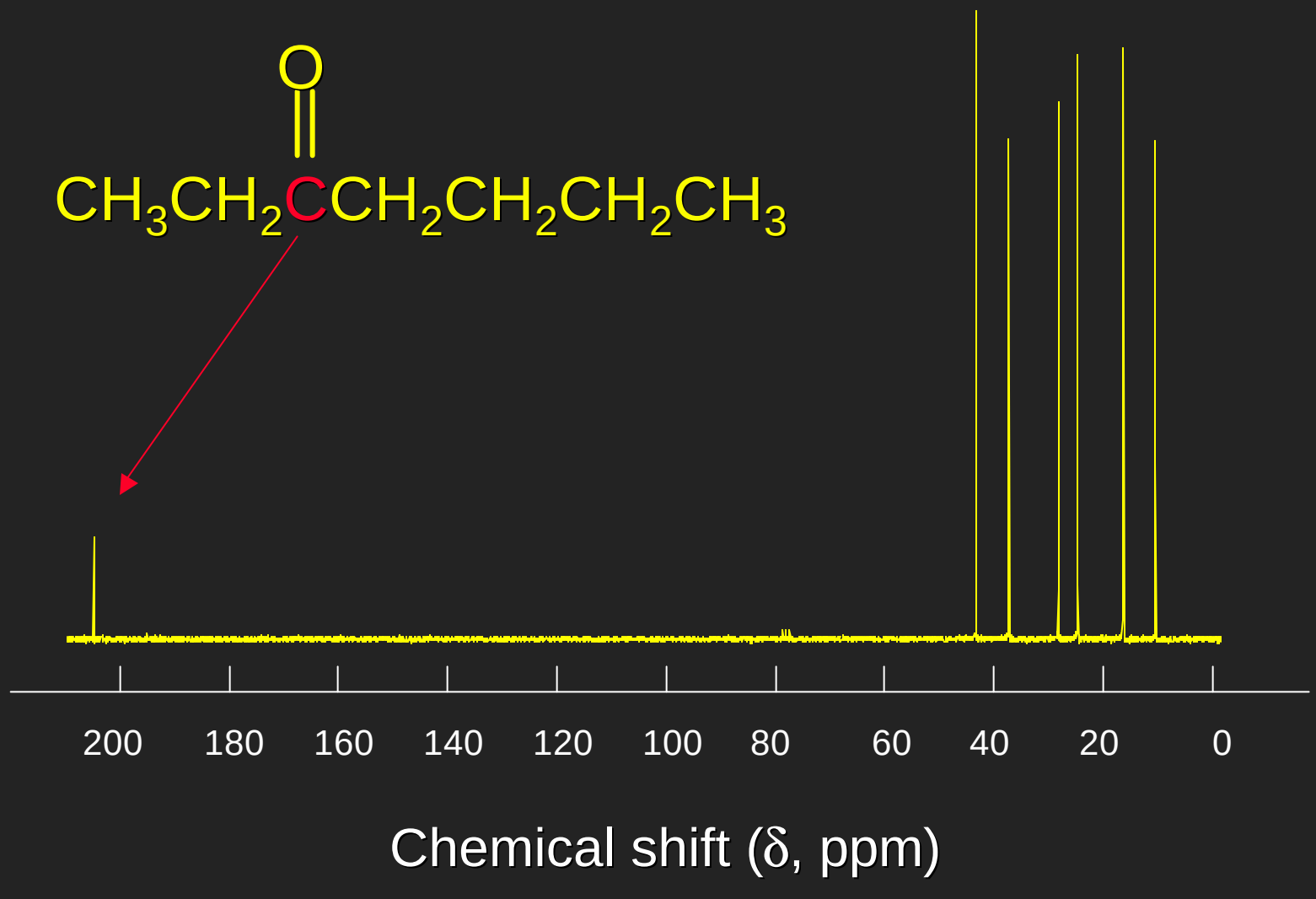

O
CH3CH2—C—CH3
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
Chemical shift (δ, ppm)

^{13}C NMR

Carbonyl carbon is at extremely low field-near δ 200 ppm

Intensity of carbonyl carbon is usually weak

Figure 17.16


O
CH3CH2CCH2CH2CH2CH3
200
180
160
140
120
100
80
60
40
20
0
Chemical shift (δ, ppm)

UV-VIS

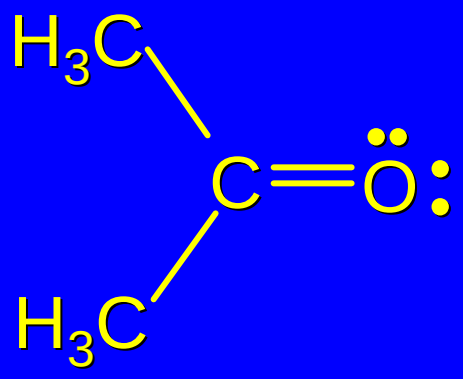
Aldehydes and ketones have two bands in the UV region:

$p \varnothing p^*$ and $n \varnothing p^*$

$p \varnothing p^*$: excitation of a bonding p electron to an antibonding p^* orbital

$p \varnothing p^*$: excitation of a nonbonding electron on oxygen to an antibonding p^* orbital

UV-VIS

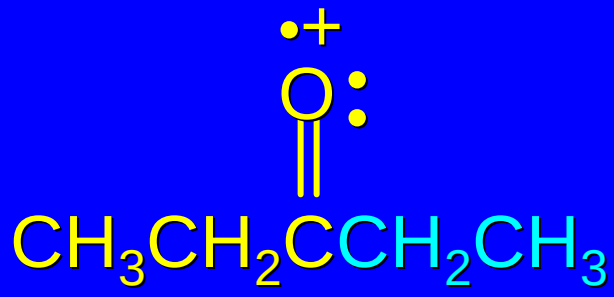


$p \varnothing p^*$ λ_{max} 187 nm

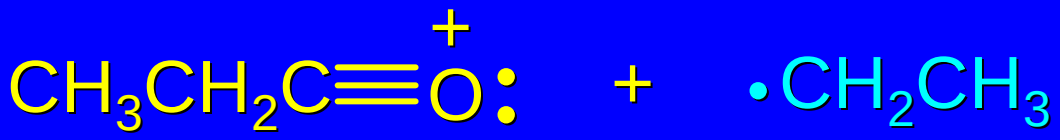
$n \varnothing p^*$ λ_{max} 270 nm

Mass Spectrometry

Molecular ion fragments to give an acyl cation



m/z 86



m/z 57