

Section 24.15
Spectroscopic Analysis of Phenols

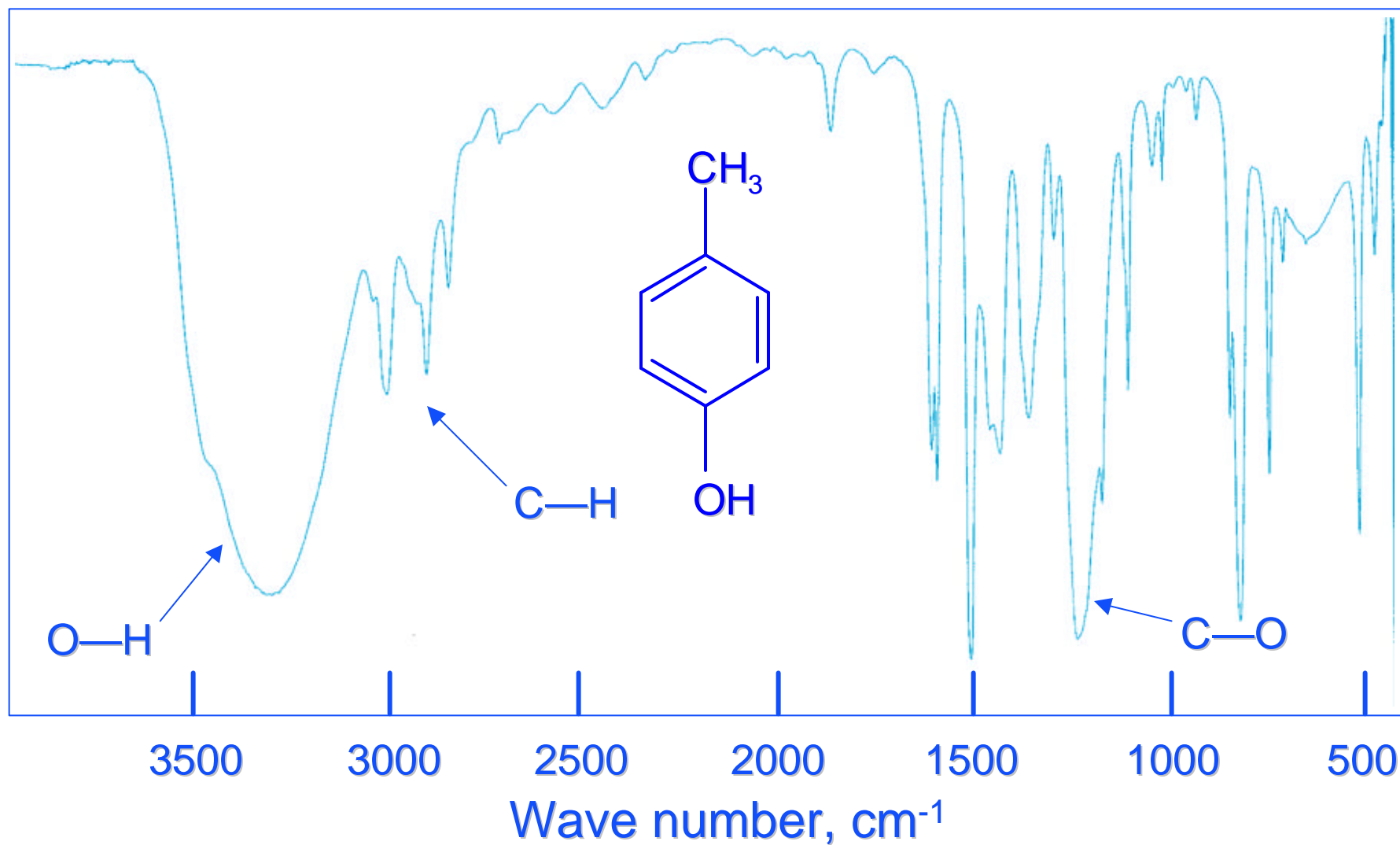
Infrared Spectroscopy

infrared spectra of phenols combine features of alcohols and aromatic compounds

O—H stretch analogous to alcohols near 3600 cm^{-1}

C—O stretch at $1200\text{-}1250\text{ cm}^{-1}$

Figure 24.3: Infrared Spectrum of p-Cresol



^1H NMR

Hydroxyl proton of OH group lies between alcohols and carboxylic acids; range is *ca.* δ 4-12 ppm (depends on concentration). For *p*-cresol the OH proton appears at δ 5.1 ppm (Figure 24.4).

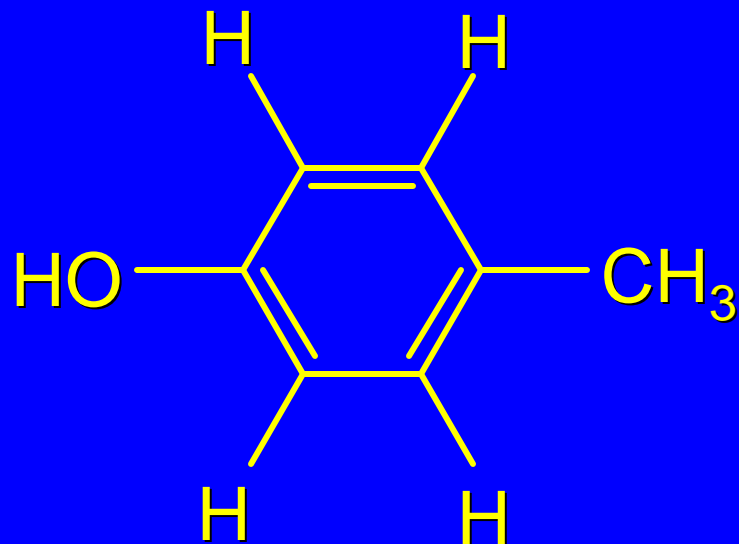
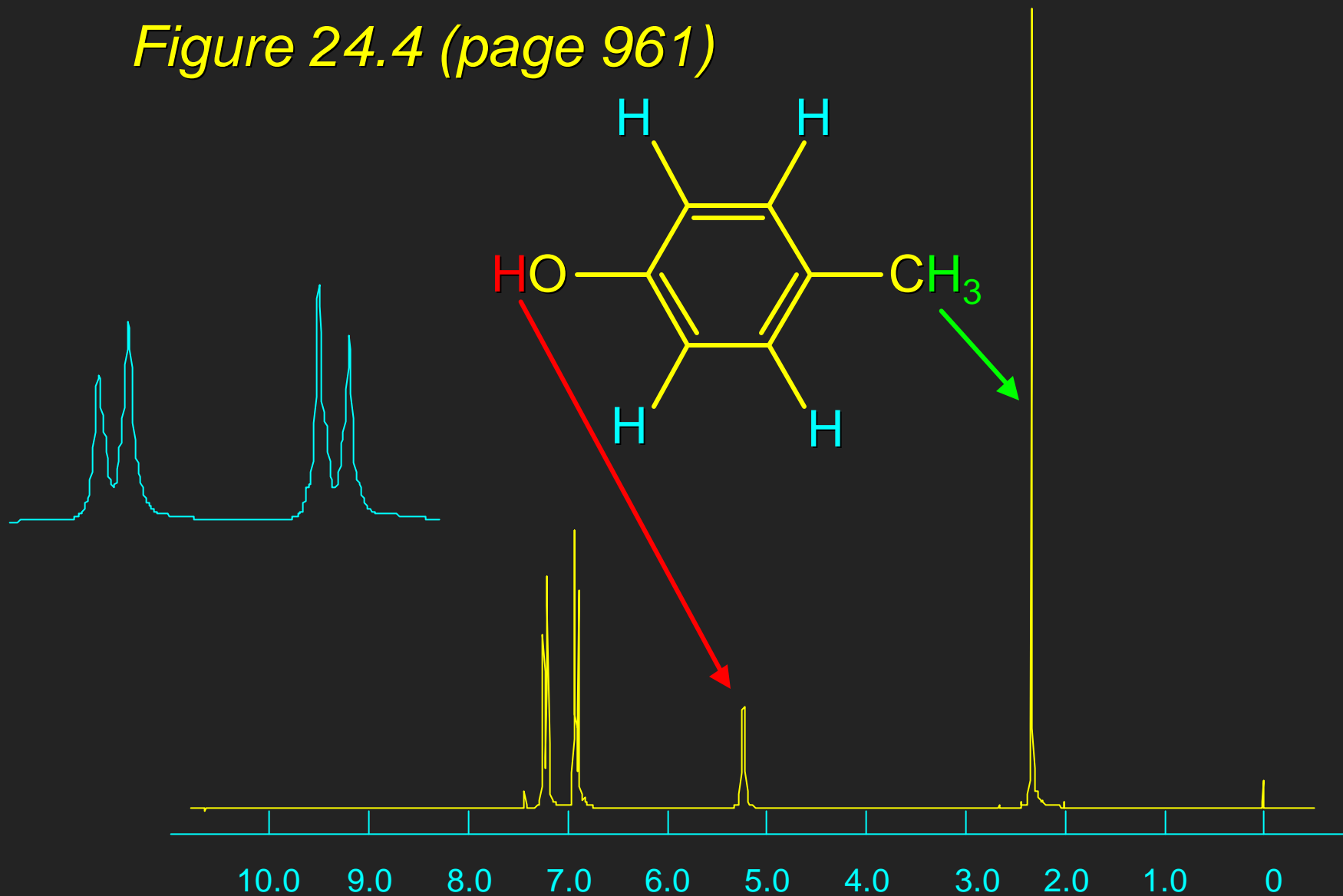
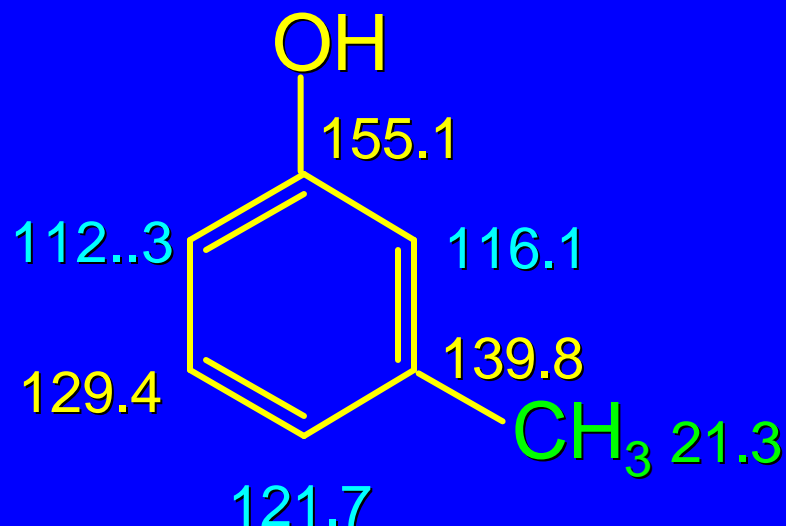


Figure 24.4 (page 961)



Chemical shift (δ, ppm)

^{13}C NMR

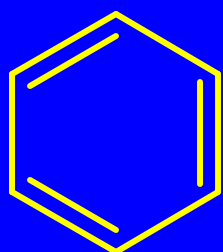


Oxygen of hydroxyl group deshields carbon to which it is directly attached.

The most shielded carbons of the ring are those that are ortho and para to the oxygen.

UV-VIS

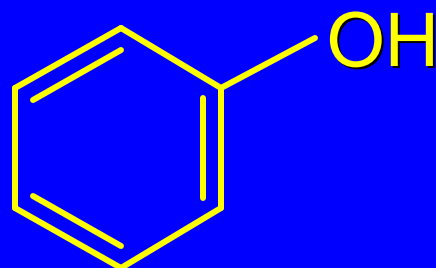
Oxygen substitution on ring shifts λ_{max} to longer wavelength; effect is greater in phenoxide ion.



λ_{max}

204 nm

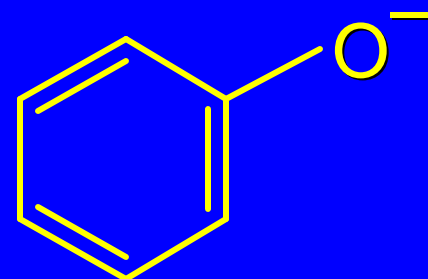
256 nm



λ_{max}

210 nm

270 nm



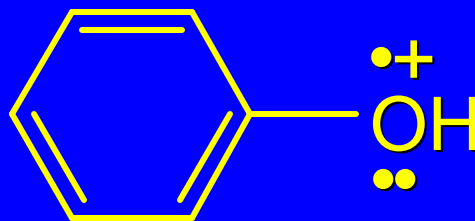
λ_{max}

235 nm

287 nm

Mass Spectrometry

Prominent peak for molecular ion. Most intense peak in phenol is for molecular ion.



m/z 94