

IR spectra in this handout were obtained from Organic Chemistry, 2<sup>nd</sup> Ed. by Fox & Whitesell & from Spectrometric Identification of Organic Compounds, 4<sup>th</sup> Ed. Silverstein, Bassler, and Morrill, John Wiley & Sons, 1981.

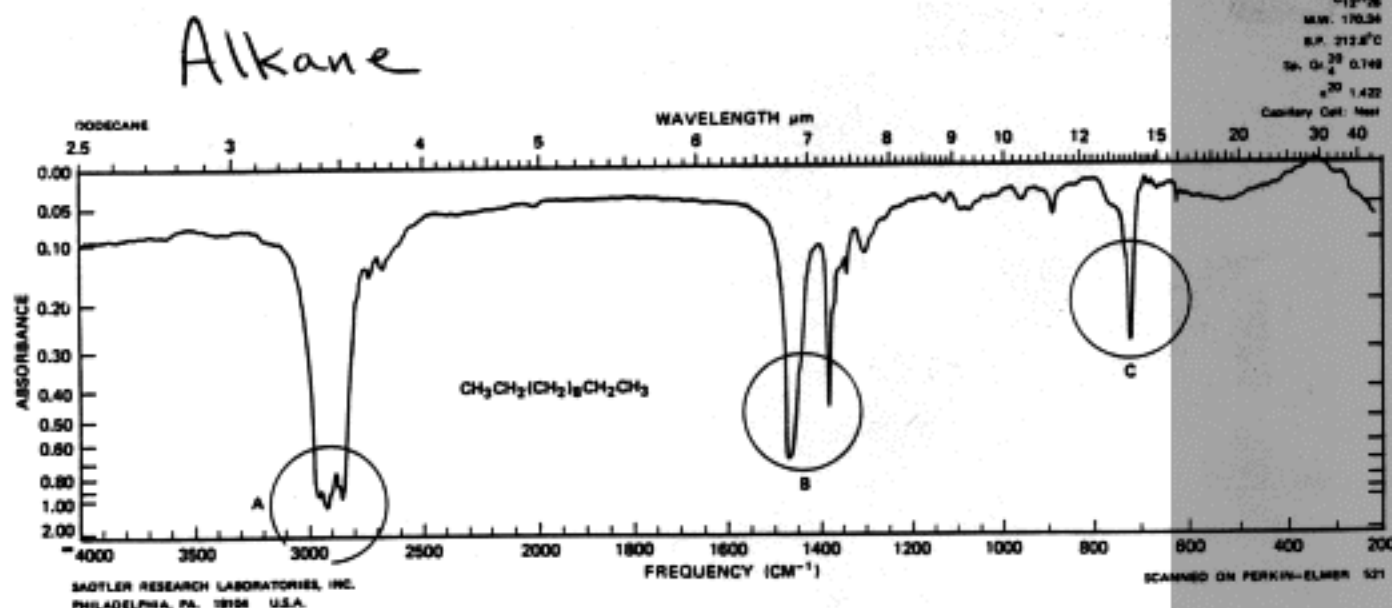


Figure 8. A. C-H stretch:  $2962\text{ cm}^{-1}$  ( $3.38\ \mu\text{m}$ )  $\nu_{\text{as}}\text{ CH}_3$ ,  $2872\text{ cm}^{-1}$  ( $3.48\ \mu\text{m}$ )  $\nu_s\text{ CH}_3$ ,  $2926\text{ cm}^{-1}$  ( $3.43\ \mu\text{m}$ )  $\nu_{\text{as}}\text{ CH}_2$ ,  $2853\text{ cm}^{-1}$  ( $3.51\ \mu\text{m}$ )  $\nu_s\text{ CH}_2$ . B. C-H bend:  $1465\text{ cm}^{-1}$  ( $6.83\ \mu\text{m}$ )  $\delta_s\text{ CH}_2$ ,  $1450\text{ cm}^{-1}$  ( $6.90\ \mu\text{m}$ )  $\delta_{\text{as}}\text{ CH}_3$ ,  $1375\text{ cm}^{-1}$  ( $7.28\ \mu\text{m}$ )  $\delta_s\text{ CH}_3$ . C.  $\text{CH}_2$  rock:  $722\text{ cm}^{-1}$  ( $13.9\ \mu\text{m}$ )  $\rho\text{ CH}_2$ .

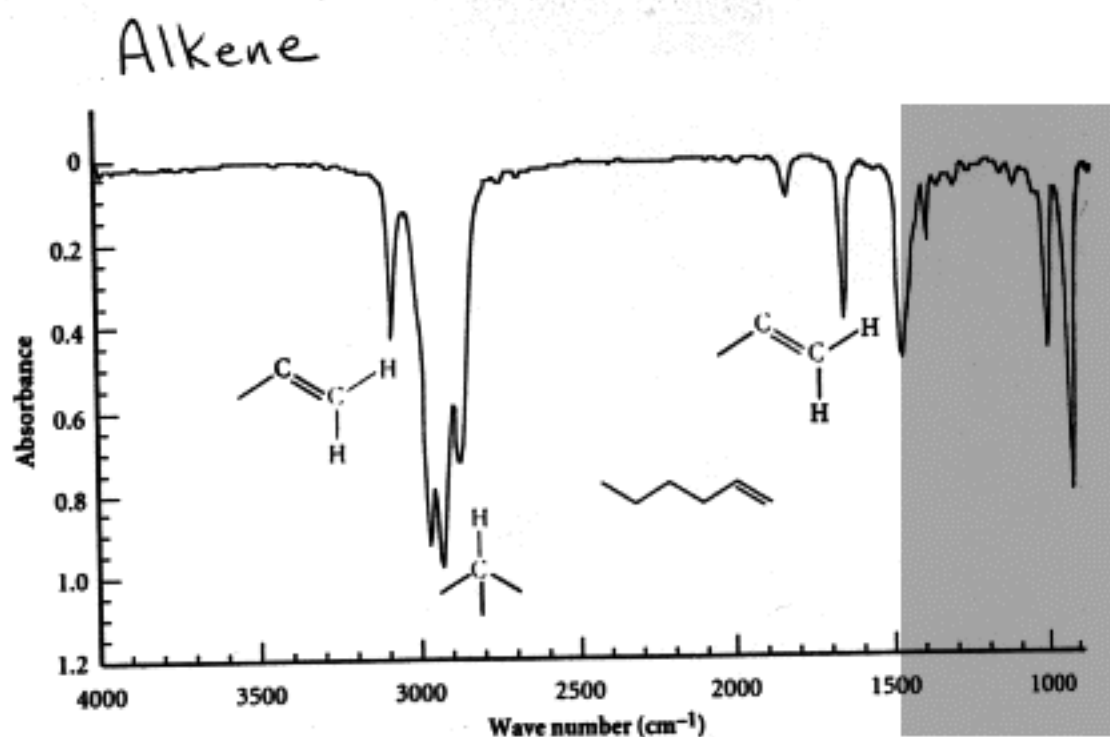


FIGURE 4.34

Ir. ed spectrum of 1-hexene.

# Alkyne

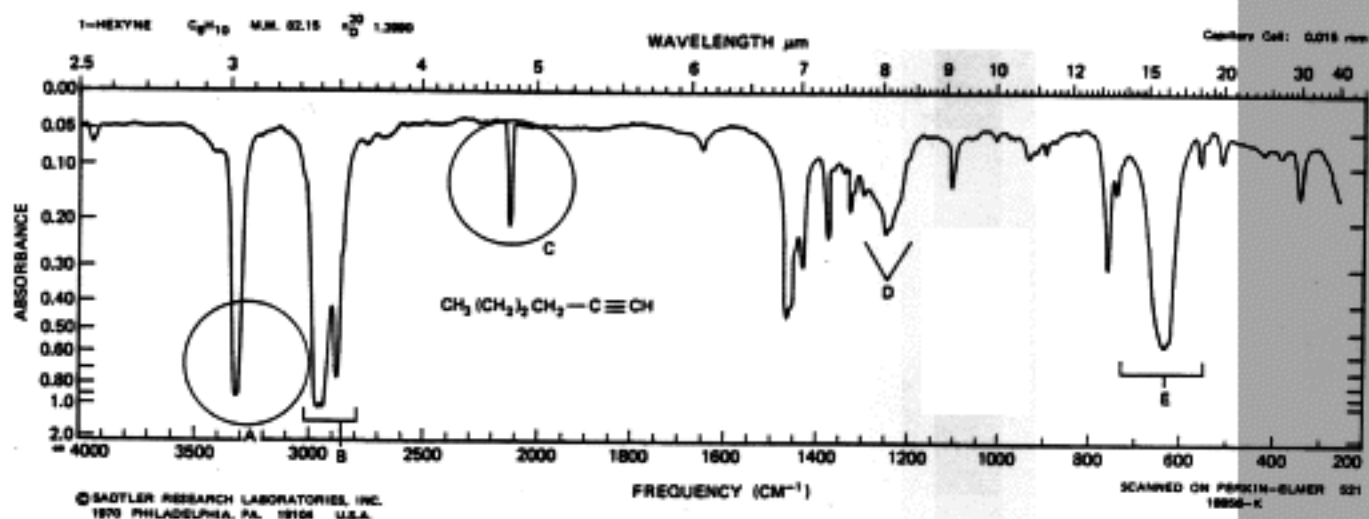


Figure 12. A.  $\equiv C-H$  stretch,  $3268\text{ cm}^{-1}$  ( $3.06\ \mu m$ ). B. Normal  $C-H$  stretch (see Figure 8),  $2857-2941\text{ cm}^{-1}$  ( $3.4-3.5\ \mu m$ ). C.  $C\equiv C$  stretch,  $2110\text{ cm}^{-1}$  ( $4.74\ \mu m$ ). D.  $\equiv C-H$  bend overtone,  $1247\text{ cm}^{-1}$  ( $8.02\ \mu m$ ). E.  $\equiv C-H$  bend fundamental,  $630\text{ cm}^{-1}$  ( $15.87\ \mu m$ ).

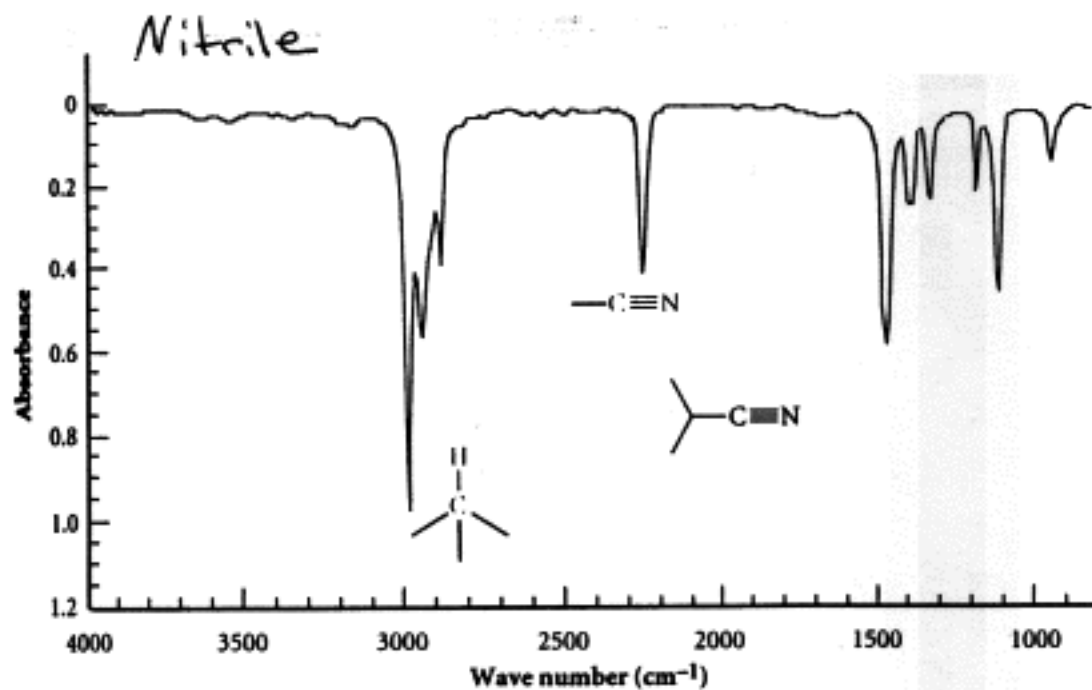


FIGURE 4.37

Infrared spectrum of isobutyronitrile.

# Alcohol

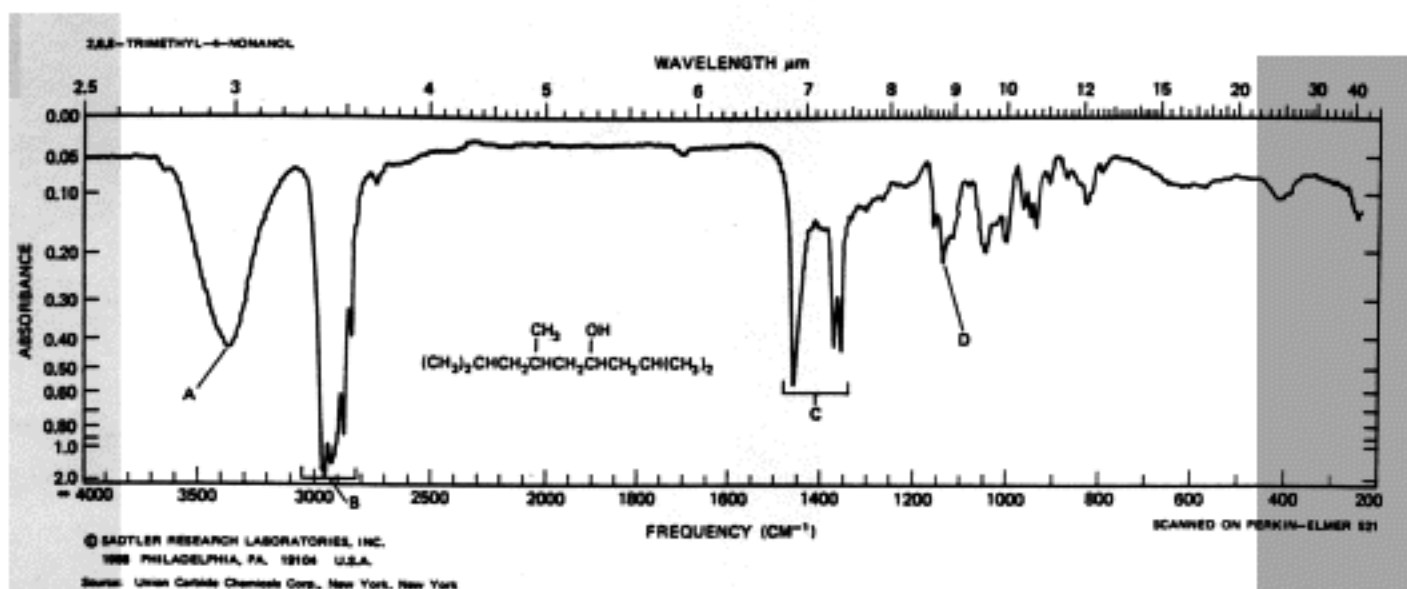


Figure 15. A. O-H stretch, intermolecular hydrogen bonding  $3355\text{ cm}^{-1}$  ( $2.98\ \mu\text{m}$ ). B. C-H stretch (see Figure 8),  $3000\text{-}2800\text{ cm}^{-1}$  ( $3.33\text{-}3.57\ \mu\text{m}$ ). C. C-H bend (see Figure 8). Note the pair of bands for the gem di-methyl groups at  $1373$  and  $1355\text{ cm}^{-1}$  ( $7.28$  and  $7.39\ \mu\text{m}$ ). D. C-O stretch  $1138\text{ cm}^{-1}$ , ( $8.79\ \mu\text{m}$ ). This appears to be weak only because the C-H bands are very intense due to the large number of C-H bonds in the molecule.

# Phenol

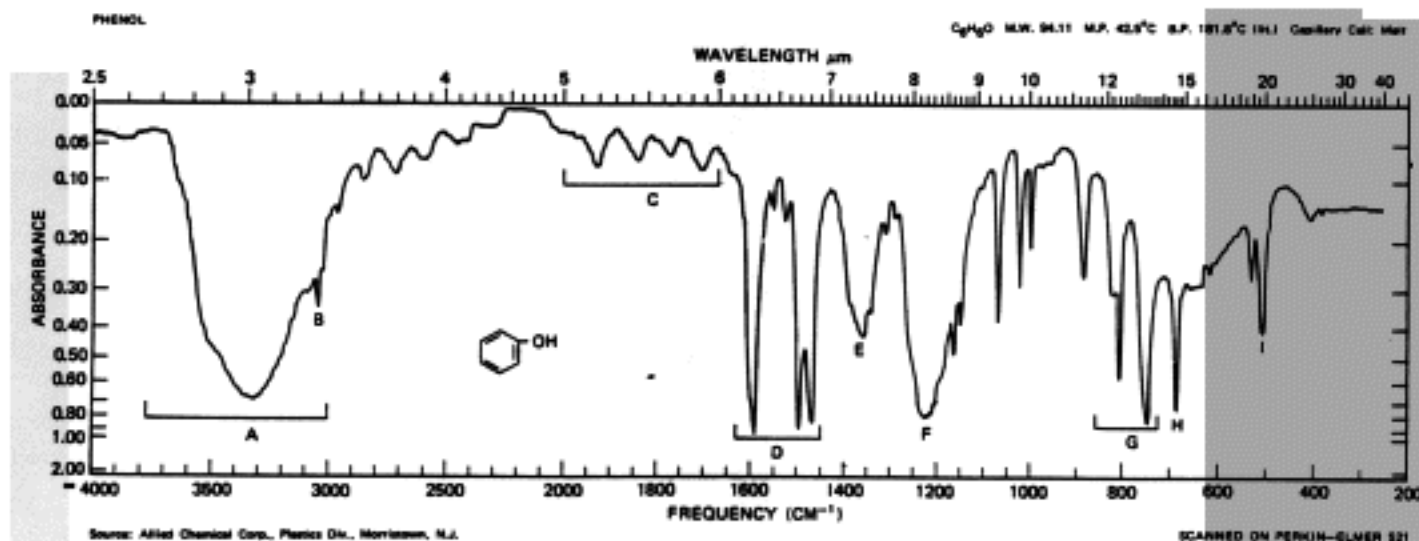


Figure 16. A. Broad, intermolecular hydrogen bonded, O-H stretch,  $3333\text{ cm}^{-1}$  ( $3.0\ \mu\text{m}$ ). B. Aromatic C-H stretch,  $3045\text{ cm}^{-1}$  ( $3.28\ \mu\text{m}$ ). C. Overtone or combination bands (see Figure 14),  $2000\text{-}1667\text{ cm}^{-1}$  ( $5.0\text{-}6.0\ \mu\text{m}$ ). D. C=C ring stretch,  $1580, 1495, 1468\text{ cm}^{-1}$  ( $6.33, 6.69, 6.81\ \mu\text{m}$ ). E. In plane O-H bend,  $1359\text{ cm}^{-1}$  ( $7.36\ \mu\text{m}$ ). F. C-O stretch,  $1223\text{ cm}^{-1}$  ( $8.18\ \mu\text{m}$ ). G. Out-of-plane C-H bend,  $805, 745\text{ cm}^{-1}$  ( $12.40, 13.43\ \mu\text{m}$ ). H. Out-of-plane ring C=C bend,  $685\text{ cm}^{-1}$  ( $14.60\ \mu\text{m}$ ). I. (Broad) hydrogen bonded, out-of-plane O-H bend, ca.  $650\text{ cm}^{-1}$  (ca.  $15.0\ \mu\text{m}$ ).

# Alcohol

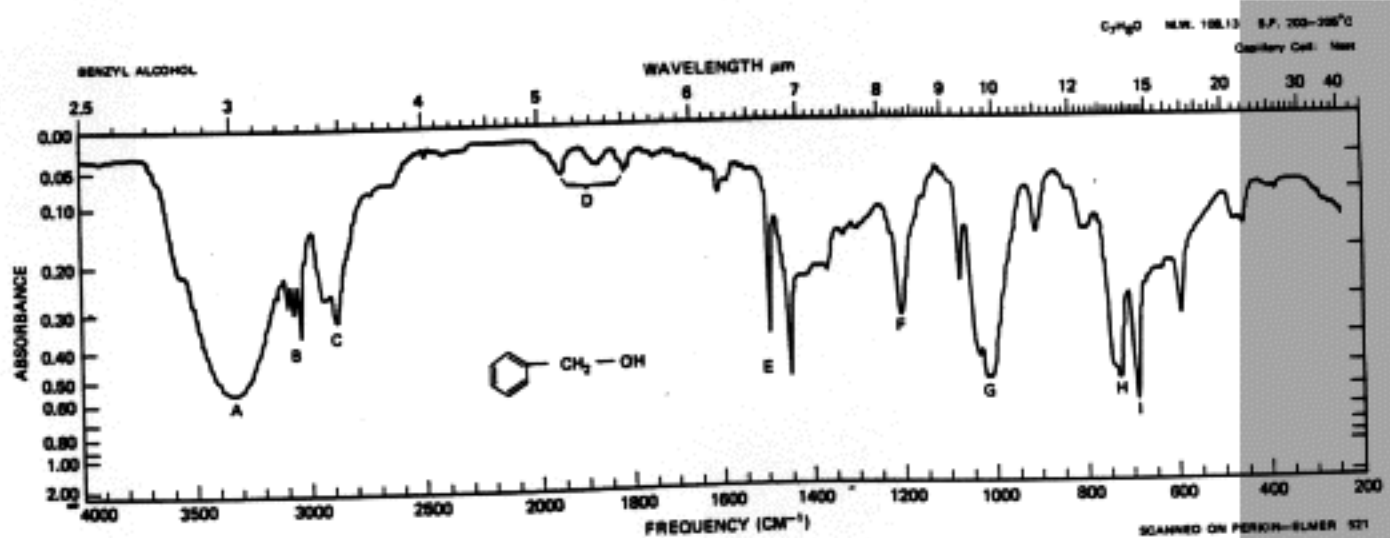
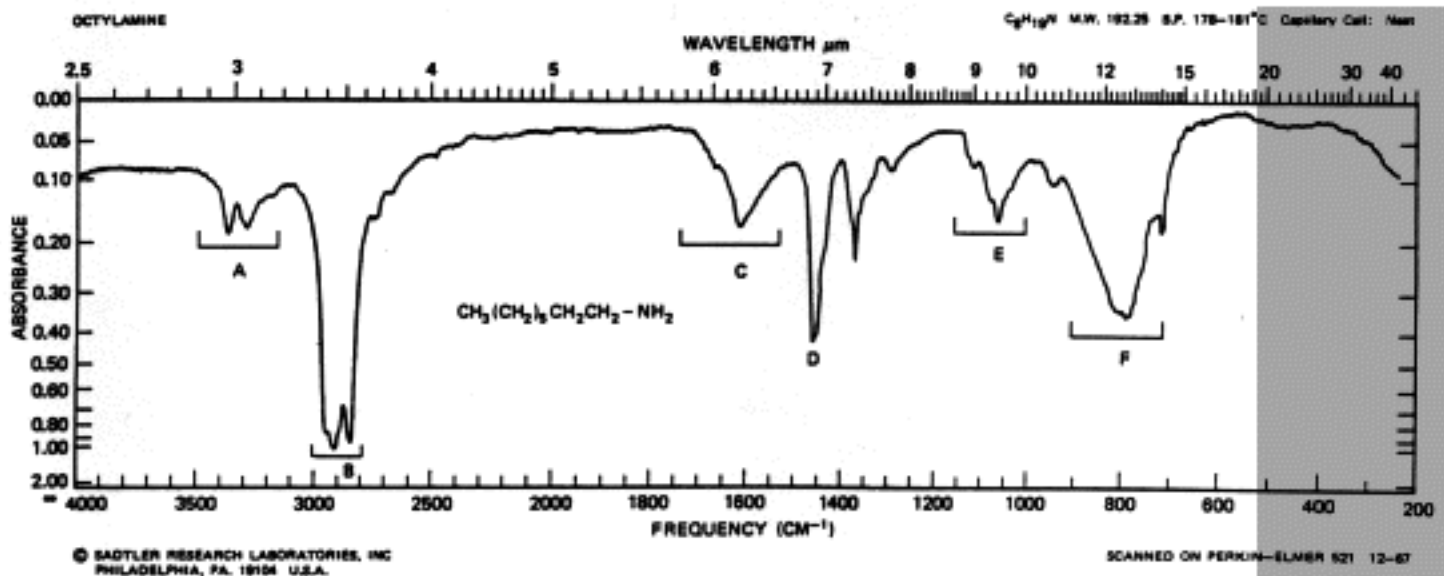


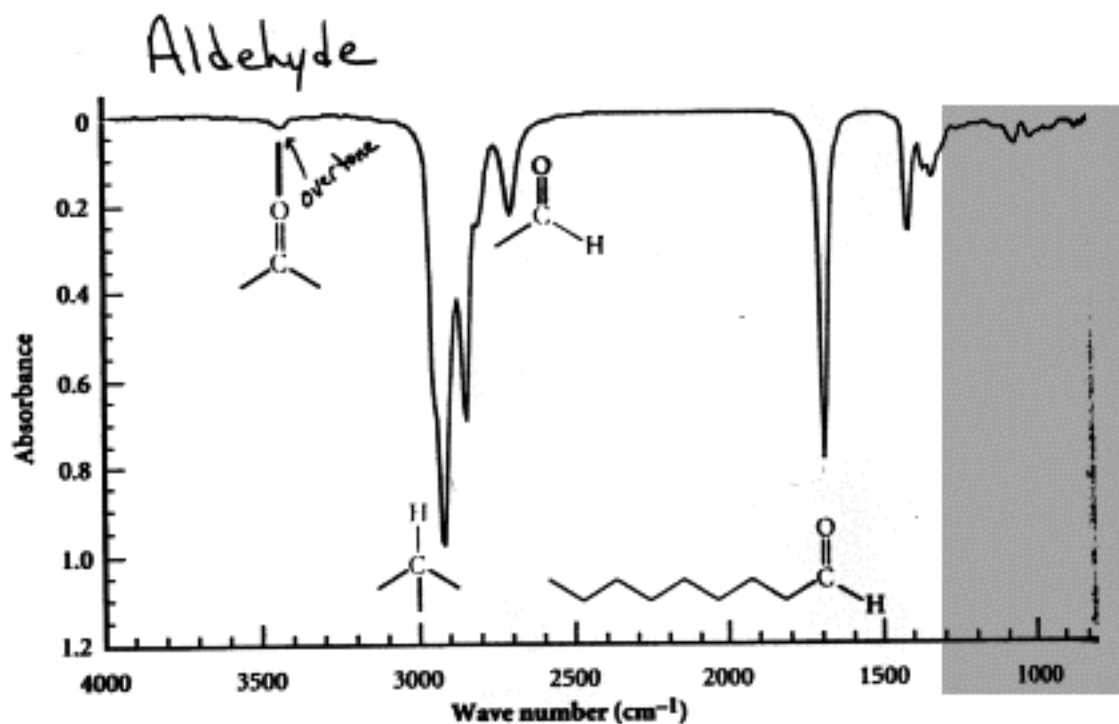
Figure 14. A. O-H stretch: intermolecular hydrogen bonded,  $3300\text{ cm}^{-1}$  ( $3.03\text{ }\mu\text{m}$ ). B. C-H stretch: aromatic  $3100\text{--}3000\text{ cm}^{-1}$  ( $3.22\text{--}3.33\text{ }\mu\text{m}$ ). C. C-H stretch: methylene,  $2980\text{--}2840\text{ cm}^{-1}$  ( $3.36\text{--}3.52\text{ }\mu\text{m}$ ). D. Overtone or combination bands,  $2000\text{--}1667\text{ cm}^{-1}$  ( $5.0\text{--}6.0\text{ }\mu\text{m}$ ). E. C=C ring stretch,  $1497, 1453\text{ cm}^{-1}$  ( $6.68, 6.88\text{ }\mu\text{m}$ ), overlapped by  $\text{CH}_2$  scissoring, ca.  $1471\text{ cm}^{-1}$  (ca.  $6.8\text{ }\mu\text{m}$ ). F. O-H bend, possibly augmented by C-H in plane bend,  $1208\text{ cm}^{-1}$  ( $8.28\text{ }\mu\text{m}$ ). G. C-O stretch, primary alcohol (see Table II)  $1017\text{ cm}^{-1}$  ( $9.83\text{ }\mu\text{m}$ ). H. Out-of-plane aromatic C-H bend,  $735\text{ cm}^{-1}$  ( $13.60\text{ }\mu\text{m}$ ). I. Ring C=C bend,  $697\text{ cm}^{-1}$  ( $14.35\text{ }\mu\text{m}$ ).

# Amine



Source: The Matheson Company, Inc., East Rutherford, N.J.

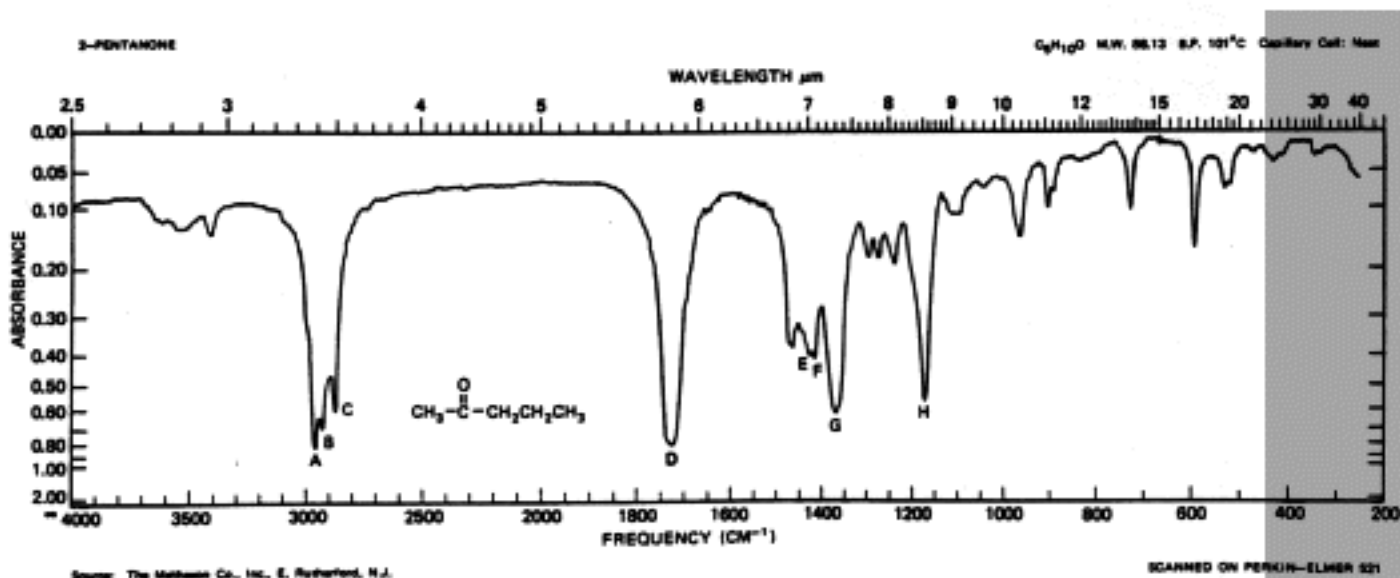
Figure 29. A. N-H stretch, hydrogen bonded, primary amine coupled doublet: Asymmetric,  $3365\text{ cm}^{-1}$  ( $2.97\text{ }\mu\text{m}$ ). Symmetric,  $3290\text{ cm}^{-1}$  ( $3.04\text{ }\mu\text{m}$ ). (Shoulder at ca.  $3200\text{ cm}^{-1}$ , ca.  $3.12\text{ }\mu\text{m}$ , Fermi resonance band with overtone of band at C.) B. Aliphatic C-H stretch,  $2910, 2850\text{ cm}^{-1}$  ( $3.44, 3.51\text{ }\mu\text{m}$ );  $\nu_s$ ,  $\text{CH}_2$ ,  $2817\text{ cm}^{-1}$  ( $3.55\text{ }\mu\text{m}$ ), see Table II, Appendix C. C. N-H bend (scissoring),  $1620\text{ cm}^{-1}$  ( $6.17\text{ }\mu\text{m}$ ). D.  $\delta_s$ ,  $\text{CH}_2$  (scissoring),  $1458\text{ cm}^{-1}$  ( $6.86\text{ }\mu\text{m}$ ), see Table II, Appendix D. E. C-N stretch,  $1063\text{ cm}^{-1}$  ( $9.41\text{ }\mu\text{m}$ ). F. N-H wag (neat sample),  $909\text{--}666\text{ cm}^{-1}$  ( $11.00\text{--}15.00\text{ }\mu\text{m}$ ).



**FIGURE 4.27**

Infrared spectrum of nonaldehyde.

## Ketone



**Figure 20.** A.  $\nu_{\text{as}}$ , methyl,  $2955 \text{ cm}^{-1}$  ( $3.39 \mu\text{m}$ ). B.  $\nu_{\text{as}}$ , methylene,  $2930 \text{ cm}^{-1}$  ( $3.41 \mu\text{m}$ ). C.  $\nu_{\text{s}}$ , methyl,  $2866 \text{ cm}^{-1}$  ( $3.49 \mu\text{m}$ ). D. Normal\* C=O stretch,  $1725 \text{ cm}^{-1}$  ( $5.80 \mu\text{m}$ ). E.  $\delta_{\text{as}}$ ,  $\text{CH}_3$ , ca.  $1430 \text{ cm}^{-1}$  (ca.  $7.0 \mu\text{m}$ ), see Table I, Appendix D. F.  $\delta_{\text{s}}$ ,  $\text{CH}_2$ , ca.  $1430 \text{ cm}^{-1}$  (ca.  $7.0 \mu\text{m}$ ), see Table II, Appendix D. G.  $\delta_{\text{s}}$ ,  $\text{CH}_3$  of  $\text{CH}_3\text{CO}$  unit,  $1370 \text{ cm}^{-1}$  ( $7.30 \mu\text{m}$ ), see Table I, Appendix D. H. C-CO-C stretch and bend,  $1172 \text{ cm}^{-1}$  ( $8.53 \mu\text{m}$ ).

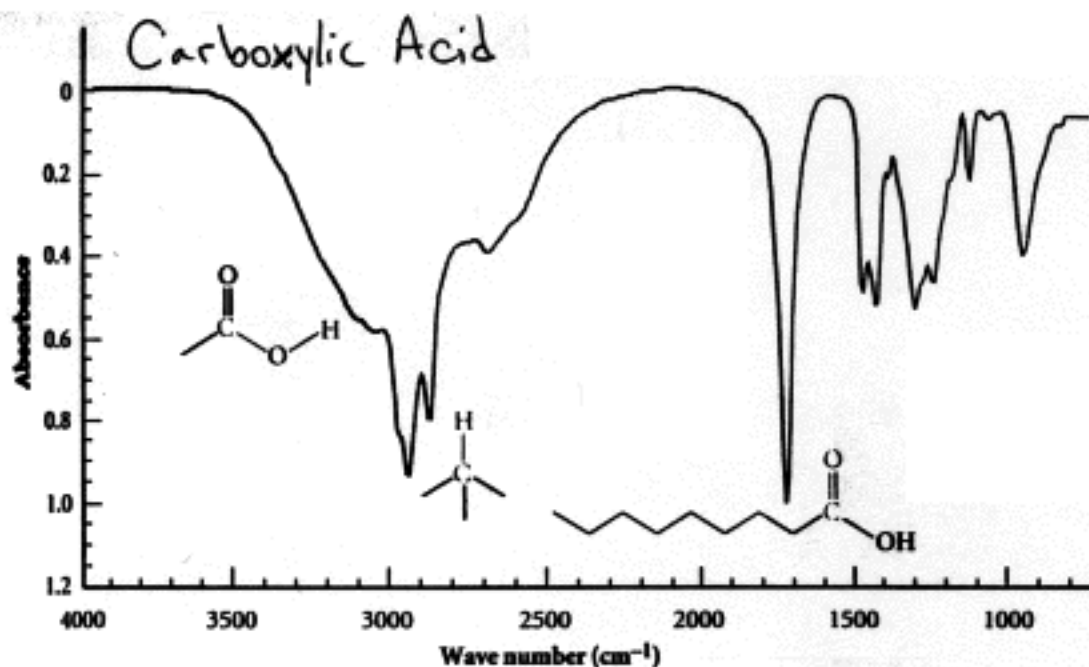


FIGURE 4.29

Infrared spectrum of nonanoic acid.

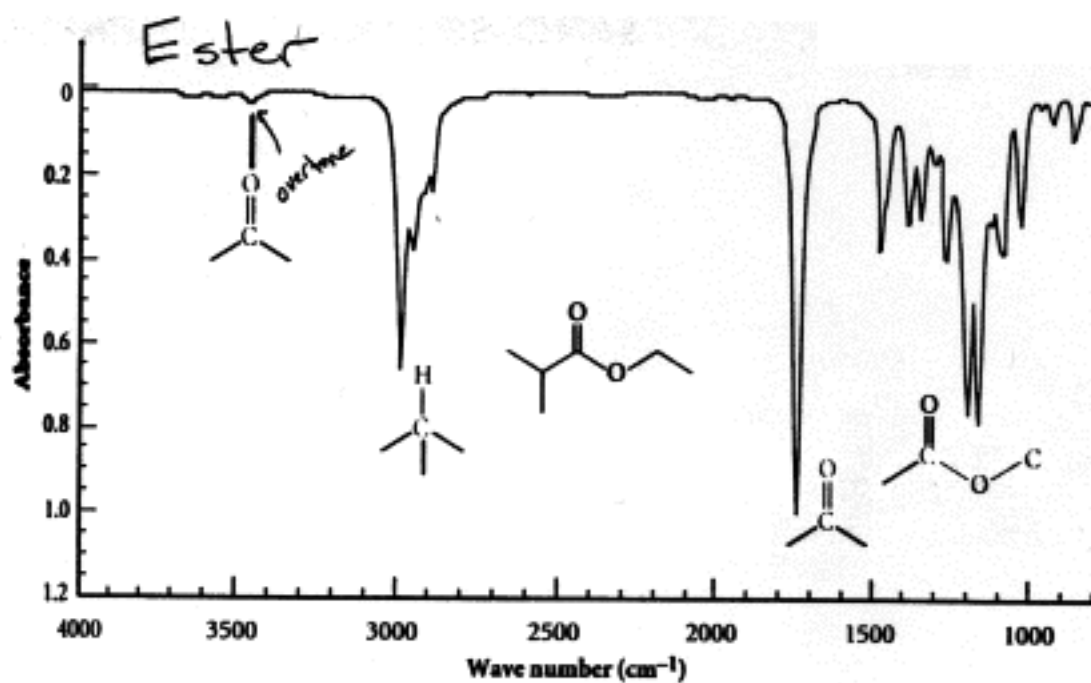


FIGURE 4.30

Infrared spectrum of ethyl isobutyrate.