

## CHARACTERISTIC INFRARED ABSORPTION BANDS

### General Trend in Bond Stretching Absorption Frequencies (in wavenumbers = $\text{cm}^{-1}$ )

|                           |                          |                          |                          |                            |
|---------------------------|--------------------------|--------------------------|--------------------------|----------------------------|
| single bonds to hydrogen: | C-H                      | N-H                      | O-H                      | 2850–3650 $\text{cm}^{-1}$ |
| triple bonds:             | $\text{C}\equiv\text{C}$ | $\text{C}\equiv\text{N}$ | $\text{C}\equiv\text{O}$ | 2000–2300 $\text{cm}^{-1}$ |
| double bonds:             | $\text{C}=\text{C}$      | $\text{C}=\text{N}$      | $\text{C}=\text{O}$      | 1500–1900 $\text{cm}^{-1}$ |
| single bonds:             | C-C                      | C-N                      | C-O                      | 800–1300 $\text{cm}^{-1}$  |

### Characteristic Absorption Bands for Common Functional Groups

| Functional Group              | Fragment                 | Mode of Vibration | Range ( $\text{cm}^{-1}$ )<br>(most useful) | Strength<br>(s,m,w,v) | Comments (typical values)                                                        |
|-------------------------------|--------------------------|-------------------|---------------------------------------------|-----------------------|----------------------------------------------------------------------------------|
| <b>Hydrocarbons:</b>          |                          |                   |                                             |                       |                                                                                  |
| <b>Alkanes</b>                | C-H                      | stretch           | <b>2850–2960</b>                            | m-s                   | nonspecific band                                                                 |
| <b>Alkenes</b>                | C=C                      | stretch           | 1640–1480                                   | v                     | (1660), substitution weakens –20 to 30 $\text{cm}^{-1}$ & stronger if conjugated |
|                               | C-H                      | stretch           | <b>3010–3100</b>                            | m                     | sharp, above 3000 $\text{cm}^{-1}$                                               |
| <b>Alkynes</b>                | $\text{C}\equiv\text{C}$ | stretch           | 2100–2260                                   | v                     | sharp, weak or gone if internal                                                  |
|                               | C-H                      | stretch           | <b>3270–3320</b>                            | s                     | sharp, stands alone                                                              |
| <b>Aromatics</b>              | ring C-C                 | overtones         | 1667–2000                                   | v                     | indicates substitution pattern                                                   |
|                               | C-H                      | stretch           | <b>3030</b>                                 | v                     | above 3000 $\text{cm}^{-1}$ characteristic bands for -OH & NH                    |
| <b>Oxygen &amp; Nitrogen:</b> |                          |                   |                                             |                       |                                                                                  |
| <b>Alcohols</b>               | O-H                      | stretch           | <b>3200–3550</b>                            | br,s                  | H-bonding in conc. Solutions                                                     |
|                               | C-O                      | stretch           | 1050–1200                                   | s                     | strong but not always easy to ID                                                 |
| <b>Ethers</b>                 | C-O                      | stretch           | 1050–1150                                   | s                     | strong but not always easy to ID                                                 |
| <b>Amines</b>                 | N-H                      | stretch           | <b>3300–3500</b>                            | m                     |                                                                                  |
|                               | 1°                       | stretch           | 3400, 3500                                  | m                     | two peaks                                                                        |
|                               | 2°                       | stretch           | 3300–3350                                   | m                     | one peak                                                                         |
| <b>Carbonyls:</b>             | C=O                      | stretch           | <b>1630–1780</b>                            | s                     | often the strongest absorption lowered by conjugation 20–30 $\text{cm}^{-1}$     |
| <b>Aldehydes</b>              | C=O                      | stretch           | 1680–1750                                   | s                     | sharp (nominally 1730)                                                           |
|                               | (CO)-H                   | stretch           | <b>2720</b>                                 | w                     | often characteristic                                                             |
| <b>Ketones</b>                | C=O                      | stretch           | 1680–1750                                   | s                     | (nominally 1715)                                                                 |
| <b>Carbox. Acid</b>           | O-H                      | stretch           | 2500–3200                                   | s                     | H-bonding, double bump, broad                                                    |
|                               | C=O                      | stretch           | 1700–1720                                   | s                     | broad range (1700)                                                               |
| <b>Esters</b>                 | C=O                      | stretch           | 1735–1750                                   | s                     |                                                                                  |
|                               | C-O                      | stretch           | 1050–1300                                   | s                     | broad, (1150–1225 if saturated)                                                  |
| <b>Amide</b>                  | N-H                      | stretch           | 3400–3500                                   | s                     | two bands for 2°, one band for 1°                                                |
|                               | C=O                      | stretch           | 1630–1690                                   | s                     | broad                                                                            |
| <b>Nitriles (CN)</b>          | $\text{C}\equiv\text{N}$ | stretch           | <b>2220–2260</b>                            | m                     |                                                                                  |

s = strong, m = medium, w = weak, v = variable

\*values in red are a good starting point\*