SURVEY OF THE IMPORTANT BONDS AND FUNCTIONAL GROUPS
IN INFRARED SPECTROSCOPY (Winter 2011 version)

Alkanes

C–H stretch 3000 – 2850 cm\(^{-1}\) (just right of 3000 cm\(^{-1}\))

C–H bend left of 1400 cm\(^{-1}\)

CH\(_3\) bend right of 1400 cm\(^{-1}\)

Alkenes

C–H stretch 3100 – 3000 cm\(^{-1}\) (just left of 3000 cm\(^{-1}\))

C–H out-of-plane (oop) bend 1000 – 650 cm\(^{-1}\)

C=C stretch 1680 – 1600 cm\(^{-1}\) (often weak)

Alkynes

C≡C stretch 2250 – 2100 cm\(^{-1}\)

C–H stretch ca 3300 cm\(^{-1}\)

Aromatics

C–H stretch 3150 – 3050 cm\(^{-1}\) (just left of 3000 cm\(^{-1}\))

C=C stretch 1650 – 1450 cm\(^{-1}\)

Weak combination and overtones 2000 – 1660 cm\(^{-1}\)

Alcohols (and phenols)

O–H stretch H-bonded 3600 – 3200 cm\(^{-1}\) (broad and medium-strong)

Free 3650 – 3600 cm\(^{-1}\) (sharp and medium; rarely observed)

C–O stretch 1300 – 1000 cm\(^{-1}\) (strong)

Amines (and amides)

N–H stretch (1\(^{\circ}\) and 2\(^{\circ}\)) 3500 – 3100 cm\(^{-1}\) (less intense and less broad than
OH; primary gives two peaks, secondary gives one peak, tertiary no peaks)

N–H bend 1640 – 1550 cm\(^{-1}\)

C–N stretch 1350 – 1000 cm\(^{-1}\)

Nitro group (NO\(_2\))

N=O stretch usually two strong peaks at 1600 – 1500 cm\(^{-1}\) and 1390 cm\(^{-1}\) –
Nitriles
\[ \text{C=NN stretch} \] near 2250 cm\(^{-1}\)

Halides
(sometimes not easy to confirm their presence with IR because of other peaks in this region)
- **Fluoride**: 1400 – 1000 cm\(^{-1}\)
- **Chloride**: 800 – 500 cm\(^{-1}\)
- **Bromide, iodide**: < 667 cm\(^{-1}\)

**CARBONYL COMPOUNDS**

**Ketones**
- \[ \text{C=O stretch} \] 1730-1700 cm\(^{-1}\) (strong)

**Aldehydes**
- \[ \text{C=O stretch} \] 1730-1700 cm\(^{-1}\) (strong)
- \[ \text{C–H stretch} \] two weak peaks at about 2750 cm\(^{-1}\) and about 2850 cm\(^{-1}\)

**Carboxylic Acids**
- \[ \text{C=O stretch} \] 1725 - 1700 cm\(^{-1}\) (strong)
- \[ \text{O–H stretch} \] very broad 3400 - 2500 cm\(^{-1}\) (will overlap with C–H stretch)
- \[ \text{C–O stretch} \] 1300 – 1200 cm\(^{-1}\)

**Esters**
- \[ \text{C=O stretch} \] 1740-1720 cm\(^{-1}\) (strong)
- \[ \text{C–O stretch} \] two peaks in 1300 – 1000 cm\(^{-1}\) usually of different intensity (can help distinguish between ester and ketone)

**Amides**
- \[ \text{C=O stretch} \] 1670 - 1640 cm\(^{-1}\) (strong)
- \[ \text{N–H stretch} \] primary amide (NH\(_2\)): two peaks at about 3350 and 3180 cm\(^{-1}\)
  Secondary amide (NH): one peak at about 3300 cm\(^{-1}\)
- \[ \text{N–H bend} \] 1640 – 1500 cm\(^{-1}\)
ABSORPTION BANDS YOU SHOULD BE ABLE TO IDENTIFY
IN AN INFRARED SPECTRUM

(As much as possible, these are given in order from left to right as they appear on a IR spectrum.)

N–H stretch  3500 – 3100 cm\(^{-1}\)
O–H stretch (alcohol or carboxylic acid) 3600 – 3200 cm\(^{-1}\) (broad and medium-strong)
C–H alkyne stretch  3300 cm\(^{-1}\)
C–H aromatic stretch  3100 – 3000 cm\(^{-1}\)
C–H alkene stretch 3100 – 3000 cm\(^{-1}\)
C–H aldehyde stretch  two weak peaks at about 2750 cm\(^{-1}\) and about 2850 cm\(^{-1}\)

C≡N stretch  2250 cm\(^{-1}\)
C≡C stretch  2250 – 2100 cm\(^{-1}\)
C=O stretch  1660-1750 cm\(^{-1}\)
C=C alkene stretch 1650 – 1450cm\(^{-1}\)
N–H bend  1640 – 1550 cm\(^{-1}\)
C–H bend  left of 1400 cm\(^{-1}\)
CH\(_3\) bend  right of 1400 cm\(^{-1}\)
N=O stretch (NO\(_2\)) usually two strong peaks at 1600 – 1500 cm\(^{-1}\) and 1390 cm\(^{-1}\) – 1300 cm\(^{-1}\)
C–O stretch  1300 – 1000 cm\(^{-1}\) (strong)