

SURVEY OF THE IMPORTANT BONDS AND FUNCTIONAL GROUPS IN INFRARED SPECTROSCOPY (Winter 2009 version)

Alkanes

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

C-H bend left of 1400 cm^{-1}

CH₃ 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 \equiv 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° and 2°) 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 (NO₂)

N=O stretch usually two strong peaks at 1600 – 1500 cm^{-1} and 1390 cm^{-1} –
1300 cm^{-1}

Nitriles

C≡N 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

C=O stretch ca 1715 cm⁻¹ (strong)

Aldehydes

C=O stretch ca 1730 cm⁻¹ (strong)

C-H stretch two weak peaks at about 2750 cm⁻¹ and about 2850 cm⁻¹

Carboxylic Acids

C=O stretch 1725 - 1700 cm⁻¹ (strong)

O-H stretch very broad 3400 - 2500 cm⁻¹ (will overlap with C-H stretch)

C-O stretch 1300 – 1200 cm⁻¹

Esters

C=O stretch ca 1735 cm⁻¹ (strong)

C-O stretch two peaks in 1300 – 1000 cm⁻¹ usually of different intensity (can help distinguish between ester and ketone)

Amides

C=O stretch 1670 - 1640 cm⁻¹ (strong)

N-H stretch primary amide (NH₂): two peaks at about 3350 and 3180 cm⁻¹
Secondary amide (NH): one peak at about 3300 cm⁻¹

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 $3500 - 3100 \text{ cm}^{-1}$

O-H stretch (alcohol or carboxylic acid) $3600 - 3200 \text{ cm}^{-1}$ (broad and medium-strong)

C-H alkyne stretch 3300 cm^{-1}

C-H aromatic stretch $3100 - 3000 \text{ cm}^{-1}$

C-H alkene stretch $3100 - 3000 \text{ cm}^{-1}$

C-H aldehyde stretch two weak peaks at about 2750 cm^{-1} and about 2850 cm^{-1}

$\text{C}\equiv\text{N}$ stretch 2250 cm^{-1}

$\text{C}\equiv\text{C}$ stretch $2250 - 2100 \text{ cm}^{-1}$

C=O stretch $1660-1750 \text{ cm}^{-1}$

C=C alkene stretch $1650 - 1450 \text{ cm}^{-1}$

N-H bend $1640 - 1550 \text{ cm}^{-1}$

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 $1600 - 1500 \text{ cm}^{-1}$ and $1390 \text{ cm}^{-1} - 1300 \text{ cm}^{-1}$

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