

Infrared Spectroscopy (IR)

What IR does

IR detects frequencies of infrared light that are absorbed by a molecule. Molecules absorb these frequencies of light because they correspond to frequencies of vibrations of bonds in the molecule.

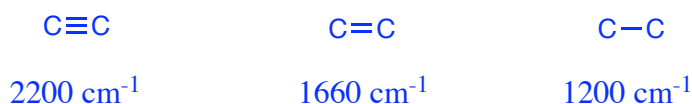
Factors that affect the frequency of light absorbed

An IR spectrometer records light absorbed from around 4000 cm^{-1} to 400 cm^{-1} . Frequencies with higher wavenumbers have more energy, while frequencies with lower wavenumbers have less energy.

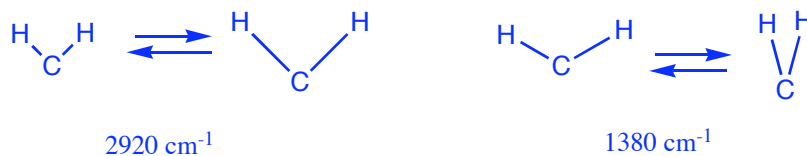
1. Bonds which have one lighter and one heavier atom vibrate faster than bonds which have two heavier atoms.



2. Stronger bonds vibrate faster than weaker bonds.

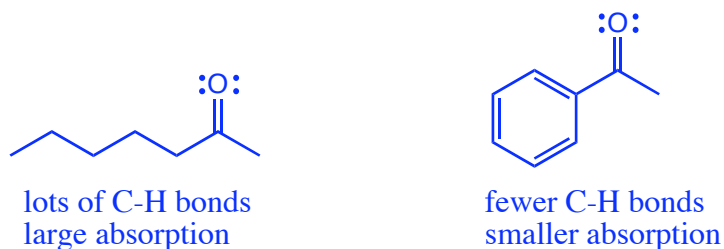


3. Stretching vibrations are faster than bending vibrations.

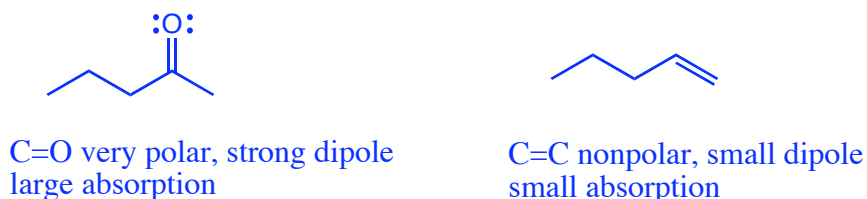


Factors that affect the amount of light that is absorbed

1. If there are many C-H bonds in a molecule absorbing light at the same frequency, the band will be much larger than if there are only a few.



2. Strength of the dipole - bonds which have a strong dipole moment will absorb light more strongly than those which have a weaker dipole moment.



Regions of the IR spectrum

Most of the bands that indicate what functional group is present are found in the functional group region, from 4000 cm^{-1} to 1300 cm^{-1} . These bands can be identified and used to determine the functional group of an unknown compound.

Bands that are unique to each molecule, like a fingerprint, are found in the fingerprint region, from 1300 cm^{-1} to 400 cm^{-1} . These bands are only used to compare the spectra of one compound to another.



Types of samples which can be used on an IR

Liquid samples:

Thin film (neat) - a few drops of the compound are placed on a transparent crystal or between two salt plates

Solid samples:

Melt - low melting point, melted between two salt plates

KBr pellet - ground with KBr, put into a press - KBr becomes transparent

Nujol mull - mush compound in a hydrocarbon oil

Bands which you can look for in an IR spectrum

Alkane

C-H sp^3 $3000\text{-}2850\text{ cm}^{-1}$

CH_2 bending $1460, 1380\text{ cm}^{-1}$

Aromatic ring

C-H sp^2 (C=C) $3000\text{-}3100\text{ cm}^{-1}$

C=C aromatic $1600\text{-}1500\text{ cm}^{-1}$

aromatic overtones (monosubstituted) $2000\text{-}1660\text{ cm}^{-1}$

Alkene

C-H sp^2 (C=C) $3100\text{-}3000\text{ cm}^{-1}$

C=C $1680\text{-}1620\text{ cm}^{-1}$

C=C bending $960\text{-}730\text{ cm}^{-1}$

Alkyne

C-H sp $\sim 3300\text{ cm}^{-1}$

$\text{C}\equiv\text{C}$ $2200\text{-}2100\text{ cm}^{-1}$

Alcohol

O-H (alcohol) 3400-3200 cm^{-1} (broad, round)
C-O 1300-1000 cm^{-1}

Carboxylic Acid

O-H (COOH) 3400-2400 cm^{-1} (very broad, overlaps C-H stretching)
C=O 1710 cm^{-1} (on benzene rings 1690-1680 cm^{-1})
COOH dimer 2700 cm^{-1} (sometimes two)

Ether

C-O 1300-1000 cm^{-1}

Ester

C=O 1800-1650 cm^{-1}
C-O 1300-1000 cm^{-1}

Anhydride

C=O 1700-1800 cm^{-1} (two prominent bands)
C-O 1300-1000 cm^{-1}

Ketone

C=O 1715-1710 cm^{-1} (on benzene rings 1690-1680 cm^{-1})

Aldehyde

C-H sp_2 (C=O) ~ 2720 cm^{-1} (sometimes 2 bands are visible)
C=O 1725-1720 cm^{-1} (on benzene rings 1700 cm^{-1})

Amine

N-H 3400-3200 cm^{-1} (not as broad as O-H) [NH_2 - 2 bands, NH - 1 band]
 NH_2 bending ~ 1600 cm^{-1} (broad); only if 1°

Amide

N-H 3400-3200 cm^{-1} (not as broad as O-H) [NH_2 - 2 bands, NH - 1 band]
 NH_2 bending ~ 1600 cm^{-1} (broad); only if 1°
C=O 1655-1650 cm^{-1}

Nitrile

$\text{C}\equiv\text{N}$ 2260-2200 cm^{-1}

Alkyl halide

C-Br 690-515 cm^{-1}
C-Cl 850-550 cm^{-1}