Examples

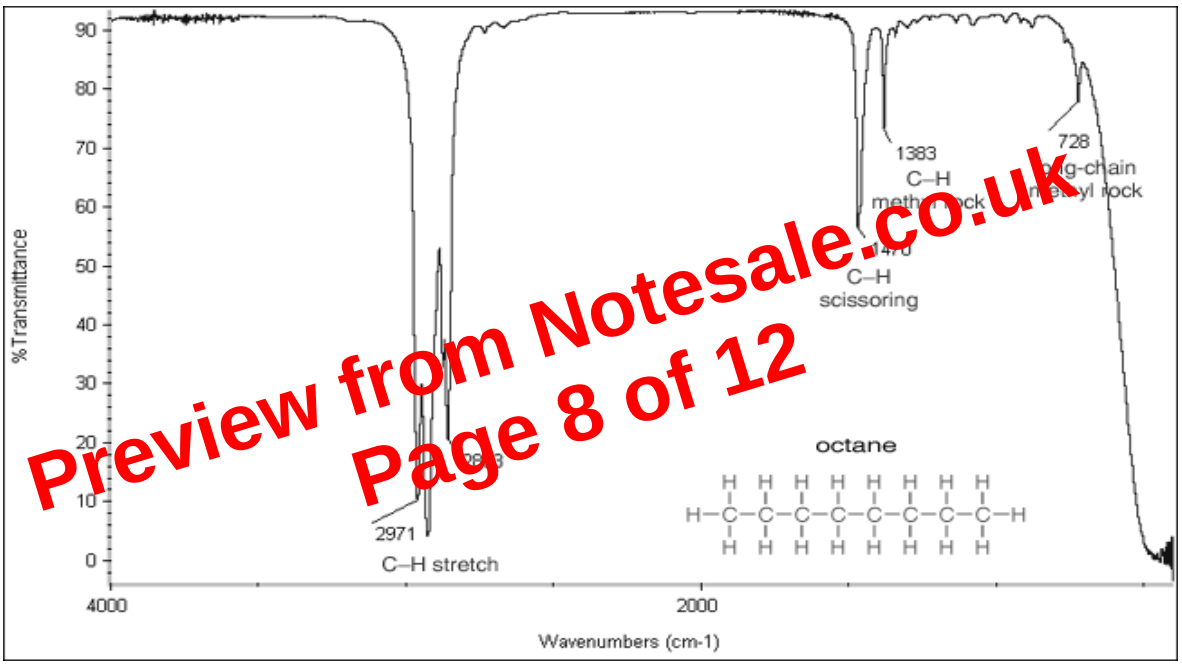
Alkanes

The spectra of simple alkanes are characterized by absorptions due to C–H stretching and bending (the C–C stretching and bending bands are either too weak or of too low a frequency to be detected in IR spectroscopy). In simple alkanes, which have very few bands, each band in the spectrum can be assigned.

- C–H stretch from 3000–2850 cm^{-1}
- C–H bend or scissoring from 1470-1450 cm^{-1}
- C–H rock, methyl from 1370-1350 cm^{-1}
- C–H rock, methyl, seen only in long chain alkanes, from 725-720 cm^{-1}

The IR spectrum of octane is shown below. Note the strong bands in the 3000-2850 cm^{-1} region due to C-H stretch. The C-H scissoring (1470), methyl rock (1383), and long-chain methyl rock (728) are noted on this spectrum. Since most organic compounds have these features, these C-H vibrations are usually not noted when interpreting a routine IR spectrum.

The region from about 1300-900 cm^{-1} is called the **fingerprint region**. The bands in this region originate in interacting vibrational modes resulting in a complex absorption pattern. Usually, this region is quite complex and often difficult to interpret; however, each organic compound has its own unique absorption pattern (or fingerprint) in this region and thus an IR spectrum be used to identify a compound by matching it with a sample of a known compound.



Alkenes

Alkenes are compounds that have a carbon-carbon double bond, –C=C–. The stretching vibration of the C=C bond usually gives rise to a moderate band in the region 1680-1640 cm^{-1}.Stretching vibrations of the –C=C–H bond are of higher frequency (higher wavenumber) than those of the –C–C–H bond in alkanes.The strongest bands in the spectra of alkenes are those attributed to the carbon-hydrogen bending vibrations of the =C–H group. These bands are in the region 1000-650 cm^{-1} (Note: this overlaps the fingerprint region).

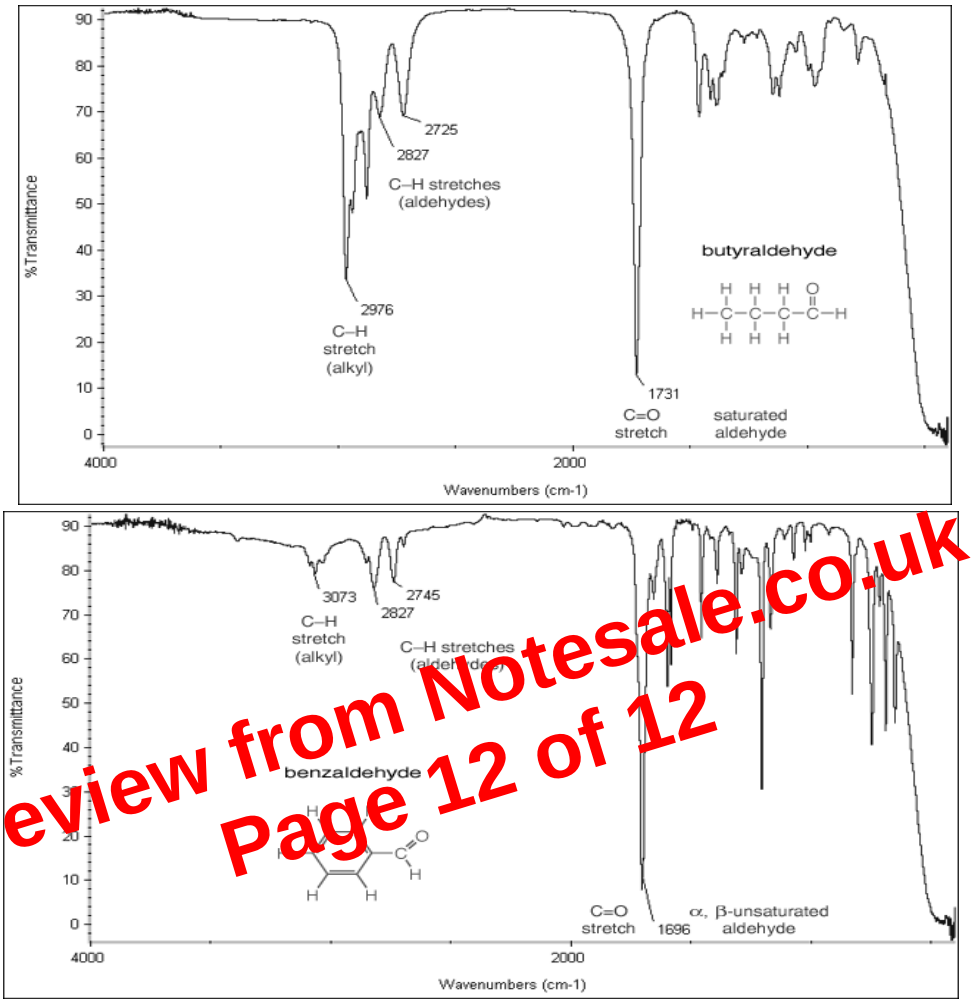
- C=C stretch from 1680-1640 cm^{-1}
- =C–H stretch from 3100-3000 cm^{-1}
- =C–H bend from 1000-650 cm^{-1}

The IR spectrum of 1-octene is shown below. Note the band greater than 3000 cm^{-1} for the =C–H stretch and the several bands lower than 3000 cm^{-1} for –C–H stretch (alkanes). The C=C stretch band is at 1644 cm^{-1}. Bands for C–H scissoring (1465) and methyl rock (1378) are marked on this spectrum; in routine IR analysis, these bands are not specific to an alkene and are generally not noted because they are present in almost all organic molecules (and they are in the fingerprint region).

- H–C=O stretch 2830-2695 cm^{-1}
- C=O stretch:
  - aliphatic aldehydes 1740-1720 cm^{-1}
  - alpha, beta-unsaturated aldehydes 1710-1685 cm^{-1}

The spectra of benzaldehyde and butyraldehyde are shown below. Note that the O=C stretch of the alpha, beta-unsaturated compound -- benzaldehyde -- is at a lower wavenumber than that of the saturated butyraldehyde.

Note the O=C–H stretches in both aldehydes in the region 2830-2695 cm^{-1}, especially the shoulder peak at 2725 cm^{-1} in butyraldehyde and 2745 cm^{-1} in benzaldehyde.



General Uses of IR spectroscopy:

- Identification of all types of organic and many types of inorganic compounds
- Determination of functional groups in organic materials
- Determination of the molecular composition of surfaces
- Identification of chromatographic effluents
- Quantitative determination of compounds in mixtures
- Nondestructive method
- Determination of molecular conformation (structural isomers) and stereochemistry (geometrical isomers)
- Determination of molecular orientation (polymers and solutions)

Common Applications:

- Identification of compounds by matching spectrum of unknown compound with reference spectrum (fingerprinting)
- Identification of functional groups in unknown substances