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1. Learning Outcomes

After studying this module, you shall be able to

- To understand the position, intensity and shape of an absorption band
- To understand the effect of bond strength on absorption frequency
- To understand how H-bonding affect the absorption band
- To know about the possible modes of vibration in aliphatic and aromatic hydrocarbons and their frequency values

2. The position of an IR-Absorption Band

The amount of energy required to stretch a bond depends on the strength of the bond and the masses of the bonded atoms. The stronger the bond, the greater the energy required to stretch it. The frequency of the vibration is inversely proportional to the mass of the atoms, so heavier atoms vibrate at lower frequencies.

The approximate vibration frequency of a bond can be calculated from the following equation derived from Hooke's law.

$$\bar{\nu} = \frac{1}{2\pi c}\sqrt{\frac{K}{\mu}}$$

Where μ is the reduced mass

And $\mu = m_1 \times m_2 / m_1 + m_2$

m_1 and m_2 are the masses of the two atoms

C is the velocity of light (2.998×10^{10} cms^{-1})

K = force constant of the bond

[For a single C-C bond, it is approximately $5 \times 10^5 gs^{-2}$ and it doubles and triples for double and triple bond respectively.]

The force constant is a measure of the strength of a bond. Thus the value of stretching frequency of a bond increases with increasing the bond strength and decreasing the reduced mass of the bonded atoms.
The triple bonds are stronger than the double bonds followed by single bonds between the same two atoms and hence vibrational frequency is in the order of triple>double>single.

$C \equiv C$	$C = C$	$C - C$
2150 cm^{-1}	1650 cm^{-1}	1200 cm^{-1}

$\xleftarrow{\hspace{2em}}$ Increasing K

As the atom attached to carbon a particular atom say carbon increases in mass, the reduced mass increases and hence the frequency of vibration decreases.

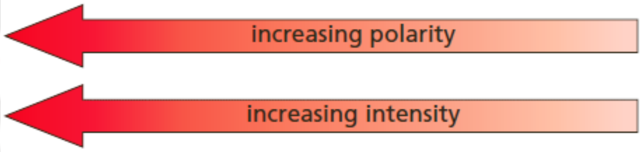
C−H	C−C	C−O	C−Cl	C−Br	C−I
3000 cm^{-1}	1200 cm^{-1}	1100 cm^{-1}	750 cm^{-1}	600 cm^{-1}	500 cm^{-1}

$\xrightarrow[\text{Increasing } \mu]{}$

3. The Intensity of Absorption Bands

The intensity of an absorption band depends on the change in the dipole moment of the bond associated with the vibration. The greater the change in dipole moment, the more intense is the absorption. The dipole moment of a bond is equal to the magnitude of the charge on one of the bonded atoms, multiplied by the distance between the two charges. If we have two different atoms, there will be an electro-negativity difference and larger the electro-negativity difference, the more intense the absorption will be. The stretching vibration of an O-H bond will be associated with a greater change in dipole moment than that of an N-H bond because O-H bond is more polar. Consequently, the stretching vibration of the O-H bond will be more intense. Likewise, the stretching vibration of an N-H bond is more intense than that of a C-H bond because the N-H bond is more polar.

O—H > N—H > C—H



The intensity of an absorption band also depends on the number of bonds responsible for the absorption. For example, if you compare the IR spectra of methane to that of octane, the octane molecule will have a much more intense C-H peak because it has many more C-H bonds than methane. The concentration of the sample used to obtain an IR spectrum also affects the intensity of the absorption bands. Concentrated samples have greater numbers of absorbing molecules and, therefore, more intense absorption bands.

4. The Shape of Absorption Bands

The shape of an absorption band can be helpful in identifying the compound responsible for an IR spectrum. For example, both O-H and N-H bonds stretch at wave numbers above 3100 cm^{-1} but the shapes of their bands are distinct. An N-H absorption band (3300 cm^{-1}) is comparatively narrower and less intense than an O-H absorption band in an alcohol and the O-H absorption band of a carboxylic acid (3300-2500 cm^{-1}) is broader than the O-H absorption band of an alcohol.

5. Factors Influencing Vibrational Frequencies

The value of vibrational frequency of a bond calculated by Hooke’s Law is not always equal to their observed value. The force constant is changed with the electronic and steric effects caused by other groups present in the surroundings. Following are some important factors affecting the vibrational frequency of a bond.

5.1 Effect of Bond Order

Bond order affects the position of absorption bands. Higher the bond order larger is the band frequency. A C-C triple bond is stronger than a C=C bond, so a C-C triple bond has higher stretching frequency than does a C=C bond. The C-C bonds show stretching vibrations in the region from 1200-800 cm^{-1} but these vibrations are weak and of little value in identifying compounds. Similarly, a C=O bond stretches at a higher frequency than does a C-O bond and a C-N triple bond stretches at a higher frequency than does a C=N bond which in turn stretches at a higher frequency than does a C-N bond.

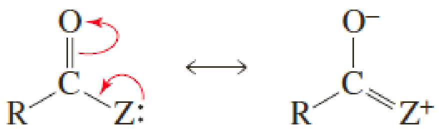
5.2 Resonance and Inductive Electronic Effects

Whenever we discuss about the IR band, a range of frequency for each stretch is usually assigned as the exact position of the absorption band depends on other structural features of the molecule, such as electron delocalization, the electronic effect of neighbouring substituents, and hydrogen bonding. Important details about the structure of a compound can be revealed by the exact position of the absorption band. For example, the IR bands for the carbonyl group in 2-pentanone, 2-cyclohexenone appears at different frequencies. The 2-Cyclohexenone absorbs at a lower frequency because the carbonyl group has less double-bond character due to electron delocalization.

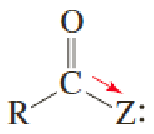
If you put an atom other than hydrogen (aldehyde) or carbon (ketone) next to the carbonyl group, it also causes the shifting of the position of the carbonyl absorption band. Whether it shifts to a lower or to a higher frequency depends on the electronic effect (inductive and mesomeric effect) of the atom.

Different substituents on carbonyl carbon changes the electronegativity of carbonyl group due to the inductive effect arises due to the different electronegativities of the carbonyl carbon and of the substituent in compounds of the type RCOZ. It involves the electrons in the sigma bonds.

The mesomeric effect involves the electrons in the pie and nonbonding orbitals and it operates in general opposite to the inductive effect. These effects cannot be isolated from one another and at a time only one of them can be applied to determine approximate results.



resonance electron donation

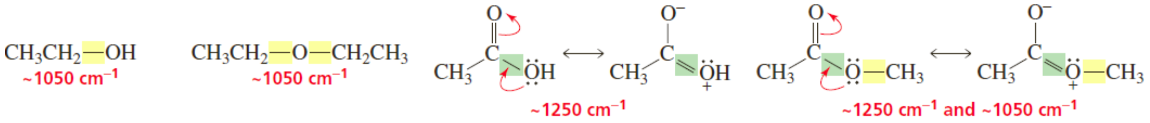


inductive electron withdrawal

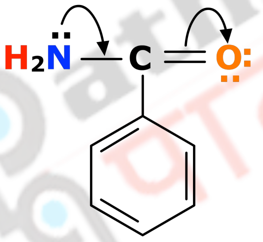
Electron releasing groups attached to the carbonyl group tend to favour the polar contribution by mesomeric effect and thus lower the bond order of the C=O bond (less double bond character) and hence resulting in a decrease of the carbonyl stretching frequency.

Electron withdrawing groups suppress the polar contribution with an effective increase in the double bond character and hence resulting in the increase of the frequency of absorption.

The predominant effect of the nitrogen of an amide is electron donation by resonance. Therefore, the carbonyl group of an amide has less double bond character than the carbonyl group of a ketone and hence amide has low C=O bond IR frequency than the ketone. In contrast, the predominant effect of the oxygen of an ester is inductive electron withdrawal, therefore the carbonyl group of an ester has more double bond character than the carbonyl group of a ketone, so the former appears at larger frequency value.

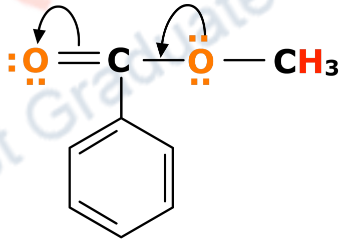


If we talk about the C-O stretching frequency it appears in the range of 1250-1050 cm^{-1}. If C-O bond is in an alcohol or in ether, the stretching frequency will be toward the lower end of the range. If this C-O bond is a part of a carboxylic group, the stretching frequency will occur at the higher end of the range. The position of the absorption varies because the bond in an alcohol is a pure single bond, whereas the bond in a carboxylic acid has partial double bond character that is due to resonance electron donation by OH group in acids. Esters show stretches at both ends of the range because esters have two single bonds, one that is a pure single bond and one that has partial double-bond character.



Benzamide

ν(C = O) 1693 cm^{-1}

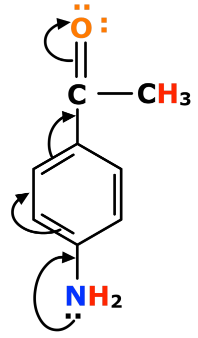


Phenyl Acetate

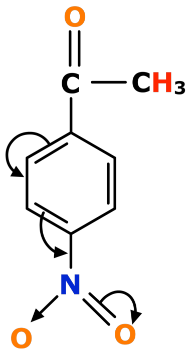
ν(C = O) 1730 cm^{-1}

In a specific example of benzamide and phenyl acetate, as the nitrogen atom is less electronegative than the oxygen atom, in amide and is more labile and participates to a greater extent in conjugation. The presence of greater degree of conjugation, C=O absorption frequency is relatively lesser than in esters.

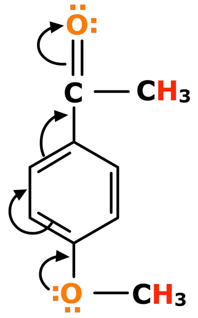
In most of the cases, mesomeric effect works along with inductive effect and cannot be ignored. It is important to note that only inductive effect is considered when the compound in meta substituted. In para substitution, both inductive and mesomeric effects become important and the domination of one over the other will decide the wavenumber of the absorption.



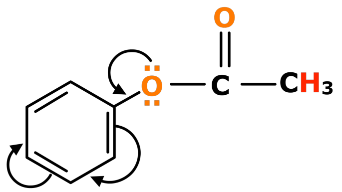
I
p-Amino Acetophenone
$\nu(C = O)$ 1677 cm^{-1}



II
p-Nitro Acetophenone
$\nu(C = O)$ 1700 cm^{-1}



III
p-Methoxy Acetophenone
ν (C = O) 1684 cm^{-1}



IV
Phenyl Acetate
$\nu(C = O)$ 1770 cm^{-1}

In the above examples, due to the low electronegativity of nitrogen atom, the lone pair of electrons participates more in conjugation in compound I as compared to that compound III. Thus, in compound I, $\nu(C=O)$ absorption occurs at lower wave number compared to that in compound III. In compounds II and IV, inductive effect dominates over mesomeric effect and hence absorption takes place at comparatively higher frequencies.

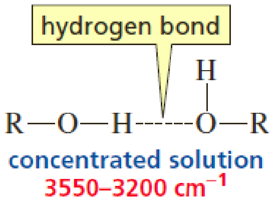
In ortho substitution, inductive effect, mesomeric effect along with steric effect is considered. In ortho substituted compounds, the lone pairs of electrons on two atoms influence each other through space interactions and change the vibrational frequencies of both the groups. This effect is called field effect.

5.3 Hydrogen Bonding

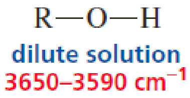
The presence of hydrogen bonding changes the position and shape of an infrared absorption band. Frequencies of both stretching as well as bending vibrations are changed because of hydrogen bonding. The X-H stretching bands move to lower frequency usually with increased intensity and band widening. The X-H bending vibration usually shifts to higher frequencies. Stronger the hydrogen bonding, greater is the absorption shift from the normal values. The two types of hydrogen bonding (intramolecular and intermolecular) can be differentiated by the use of infrared spectroscopy.

Inter-molecular hydrogen bonding involves association of two or more molecules of the same or different compound, and it may result in dimer molecules as in carboxylic acids. Intra-molecular hydrogen bonds are formed when the proton donor and acceptor are present in a single molecule under special conditions that allow the required overlap of orbitals, e.g. formation of a 5 or 6 member rings.

The extent of inter-molecular hydrogen bonding depends upon the concentration of the solution and hence the position and the shape of an absorption band also depend on the concentration of the solution. The more concentrated the solution, the more likely it is for the OH-containing molecules to form intermolecular hydrogen bonds. It is easier to stretch an O-H bond if it is hydrogen bonded, because the hydrogen is attracted to the oxygen of neighbouring molecule. Therefore, the O-H stretching of a concentrated (hydrogen bonded) solution of an alcohol occurs at about 3550 cm^{-1}, whereas the O-H stretching band of a dilute solution (with little or no hydrogen bonding) appears at 3650 cm^{-1}. Additionally, hydrogen-bonded OH groups also have broader absorption bands whereas the absorption bands of non-hydrogen–bonded OH groups are sharper.



$$R—O—H\text{------}\overset{H}{\overset{|}{O}}—R$$



Hydrogen bonding interactions can also occur between functional groups of solvent and solute. Three classes of solvent exist which may lead to trouble when used for hydrogen-bonding studies is solution. First, compounds which contain hydrogen donor groups, e.g. halogenated compounds which contain a sufficient number of halogens to activate the hydrogens present, such as chloroform. Secondly, compounds which contain non-bonded electron pairs, such as ethers, aldehydes and tertiary amines.

In addition, there are compounds which contain both types of group, e.g. water and alcohols. There are only a few solvents that do not have the above characteristics, such as carbon tetrachloride (CCl_4) and carbon disulfide (CS_2). These still contain lone electron pairs, but being on S and Cl are less available, and any interactions will be extremely weak.
Apart from the concentration and solvent effects, temperature also affects the degree of hydrogen bonding in a compound. High temperature decreases the extent of hydrogen bonding.

5.4 Fermi Resonance

Fermi resonance is a phenomenon which was first explained by the Italian physicist Enrico Fermi to account for shifting of the energies and intensities of absorption bands in an infrared spectroscopy. Sometimes, it happens that two different vibrational levels have nearly the same energy. If such vibrations belong to the same species of molecules, then a mutual perturbation of energy may occur, resulting in the shift of one towards lower frequency and the other towards a higher frequency. It is also accompanied by a substantial increase in the intensity of the respective bands.

Fermi resonance was first discovered in carbon dioxide by Fermi and it is also found in the vibrational spectra of aldehydes, where the C-H bond in the CHO group interacts with the second harmonic level, derived from the fundamental frequency of the deformation vibration of the CHO group (2*1400 cm^{-1}). The result is a Fermi doublet with branches around 2830 cm^{-1} and 2730 cm^{-1}. It is important for Fermi resonance that the vibrations connected with the two interacting levels be localized in the same part of the molecule.

5.4 Bond angles

Smaller ring requires the use of more p-character to make the internal C-C bonds for the requisite small angles. This gives more s character to the C=O sigma bond which causes the strengthening and stiffening of the exocyclic double bond. The force constant K is then increased and the absorption frequency increases.

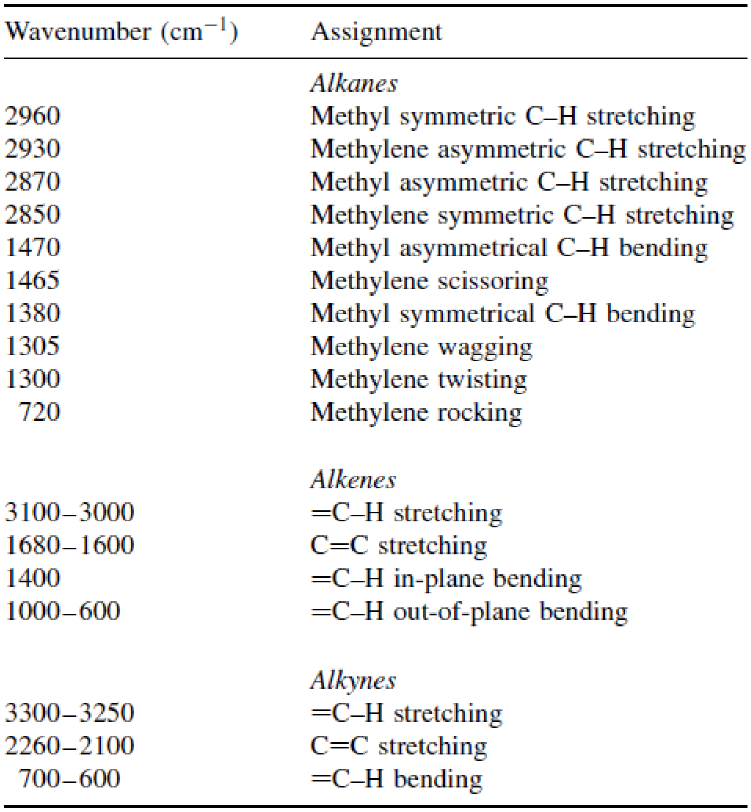
6. Characteristic absorption bands for hydrocarbons

These compounds have carbon and hydrogens only and may be saturated, unsaturated, aliphatics, cyclics and aromatics. The characteristic vibrational modes of aliphatic and aromatic hydrocarbons and their absorption frequencies are described in subsequent sections.

7. Aliphatic hydrocarbons

The stretching and bending vibrations frequencies of alkanes, alkenes and alkynes are described in table 1

Table 1: Characteristic frequencies of absorption bands for aliphatic hydrocarbons



Wavenumber (cm^{-1})	Assignment
	Alkanes
2960	Methyl symmetric C–H stretching
2930	Methylene asymmetric C–H stretching
2870	Methyl asymmetric C–H stretching
2850	Methylene symmetric C–H stretching
1470	Methyl asymmetrical C–H bending
1465	Methylene scissoring
1380	Methyl symmetrical C–H bending
1305	Methylene wagging
1300	Methylene twisting
720	Methylene rocking
	Alkenes
3100–3000	=C–H stretching
1680–1600	C=C stretching
1400	=C–H in-plane bending
1000–600	=C–H out-of-plane bending
	Alkynes
3300–3250	=C–H stretching
2260–2100	C=C stretching
700–600	=C–H bending

7.1 Alkanes

In alkanes only two types of bonds are present that is C–H and C–C bonds. The most useful bands in alkanes are those arising from C–H stretching and C–H bending. A methyl group usually shows two strong and distinct bands, one at 2960 cm^{-1} due to asymmetric stretching and the other at 2870 cm^{-1} due to symmetric stretching. While the methylene group show asymmetric stretching at 2930 cm^{-1} and symmetric stretching at 2850 cm^{-1}. The C-H bonds do not participate in H-bonding and hence the frequencies are not affected by chemical environment. The presence of several methyl groups in a molecule results in strong absorptions at these positions.

The C-H in-plane bending vibrations of a methyl group give two bands, i.e. a symmetrical band at 1380 cm−1 and an asymmetrical band at 1460 cm^{-1}. Methylene groups give rise to four bending vibrations: scissoring (1465 cm^{-1}), rocking (720 cm^{-1}), wagging (1305 cm^{-1}) and twisting (1300 cm^{-1}). The band at 1460 cm^{-1} indicates the C-H asymmetric bending of both methyl and methylene groups whereas the band at 1380 cm^{-1} represents symmetric bending of methyl group only. Thus the peak at 1380 cm^{-1} is extremely useful in detecting the presence of methyl group because this band is hardly overlapped to the absorptions due to the methylene and methane absorption bands.

The presence of two or more methyl groups, attached to the same carbon atom results in splitting of the C-H symmetric bending vibrations. For example the isopropyl group gives rise to two bands 1397 cm^{-1} and 1370 cm^{-1} and in t-butyl group the two bands appear at 1385 cm^{-1} and 1370 cm^{-1} (Figure 1).

The methine C-H shows C-H stretching and bending vibrations at 2890 cm^{-1} and 1340 cm^{-1} respectively and are very weak with no practical significance (Figure 1).

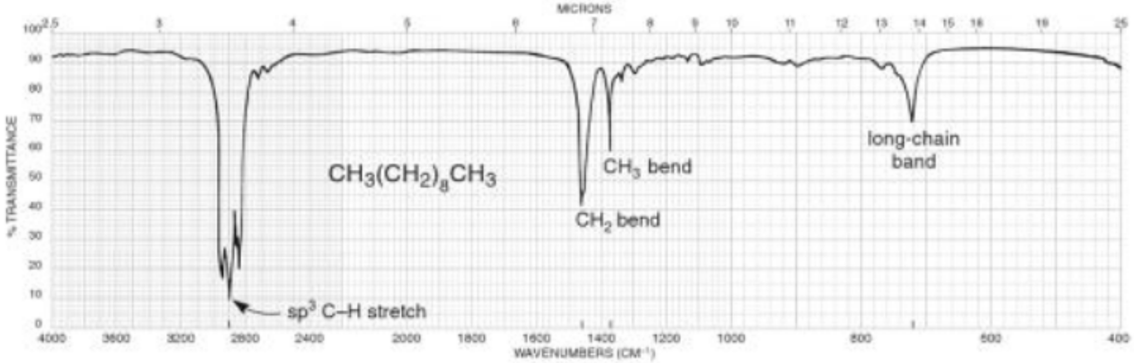


Figure 1: IR-spectrum of decane

7.2 Cycloalkanes

In case of unstrained cycloalkanes, the C-H stretching frequencies are the same (2800 – 3000 cm^{-1}) as in the case of acyclic compounds. However, methylene scissoring bands shift slightly to smaller wavenumber (1470 cm^{-1} in hexane and 1448 cm^{-1} in cyclohexane). In sterically strained cyclic compounds, the C-H stretching normally occurs at slightly higher frequencies. For example the ring CH_2 and CH groups in a monoalkyl cylcopropane ring absorb in the range of 3100-2990 cm^{-1}.

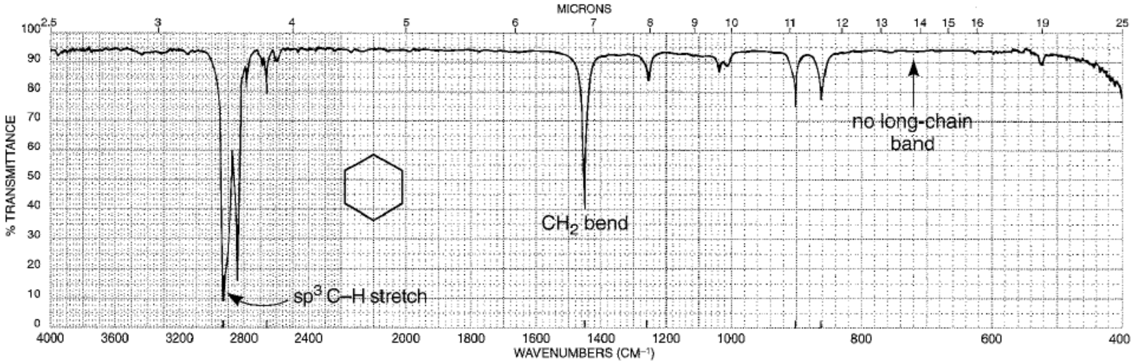


Figure 2: IR-spectrum of cyclohexane

Methylene C-H in-plane bending vibrations in cyclic alkenes shift slightly to smaller frequency as compared to their acyclic counterparts. For example, cyclohexane absorb at 1452 cm^{-1} whereas n-hexane absorb at 1468 cm^{-1}. The C-C bond vibrations appear as weak bands in 1200-800 cm^{-1} region and are seldom used for structural study. Whereas the C-C bending absorptions occur at < 500 cm^{-1} and are usually below the range of IR instrument (Figure 2)

7.3 Alkenes

There are four major bands associated with alkene molecular framework. These are the out-of-plane and in-plane =C–H bending, C=C stretching and =C–H stretching. In completely symmetrical alkenes, such as ethylene, tetrachloroethylene etc., C=C stretching band is absent, due to lack of change in dipole moment in completely symmetrical molecule. On the other hand, non-symmetrically substituted double bonds exhibit strong absorption bands.

Olefinic C-H stretching occurs near 3100-3000 cm^{-1}. C=C stretching band occurs near 1680-1600 cm^{-1}. The C=C absorption bands are more intense for *cis* isomers than for trans isomers. Also, terminal olefins show stronger C=C double bond stretching vibrations than internal double bonds. Conjugation moves C=C stretching bands towards lower frequency with increased intensity than in comparison to non-conjugated ones. In case of olefins, conjugated with an aromatic ring, the C=C stretching appears at 1625 cm^{-1} (s) and an additional band at ~1600 cm^{-1} is observed due to aromatic double bond.

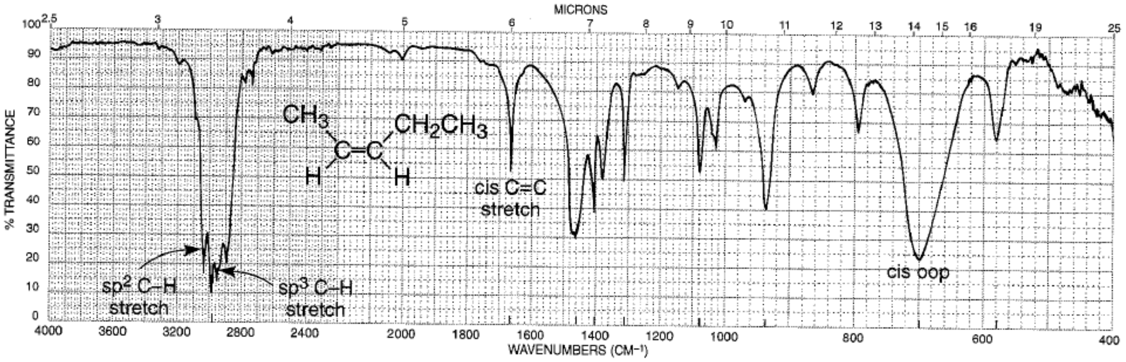


Figure 3: IR-spectrum of Cis-2-pentene

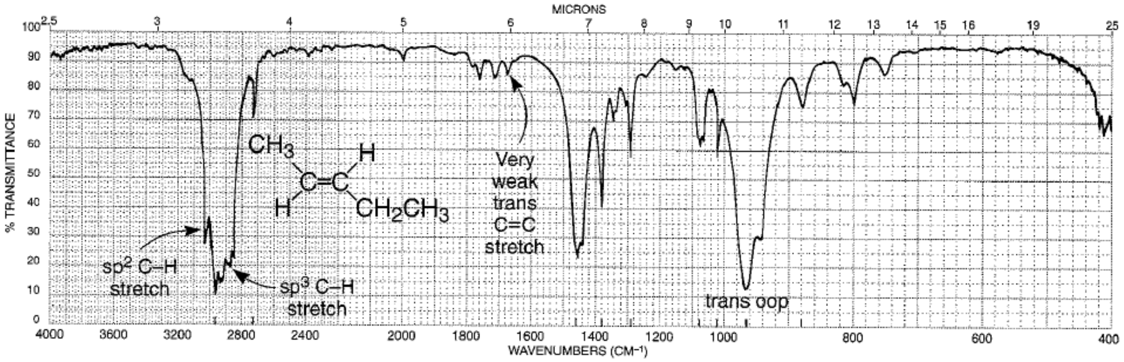


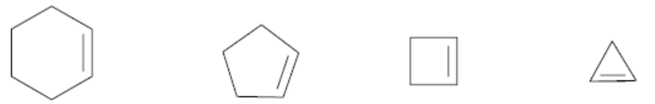
Figure 4: IR-spectrum of trans-2-pentene

The =C-H in-plane bending vibrations occur near 1400 cm^{-1} whereas the =C-H out-of-plane bending band occur in the range from 1000-680 cm^{-1} (Figure 3,4).

Note: In compounds containing both olefinic and alkyl C-H bonds, the bands above 3000 cm^{-1} are generally attributed to aromatic or aliphatic C-H stretching, whereas between 3000-2840 cm^{-1} are generally assigned to the alkyl C-H stretching.

7.4 Cycloalkenes

The absorption frequency of a double bond in a cyclic ring is very sensitive to ring size. The absorption frequency decreases as the internal bond angle decreases and is becomes lowest in cyclobutene (90^{o} angle) but after that the frequency increases again for cyclopropene (Figure 5).



Cyclohexene 1646 cm^{-1}

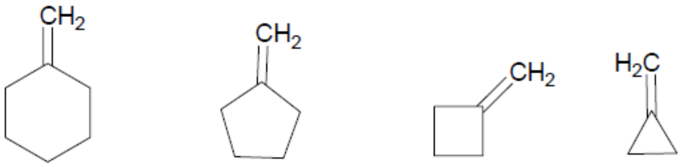
Cyclopenetene 1611 cm^{-1}

Cyclobutene 1566 cm^{-1}

Cycloprpene 1656 cm^{-1}

Figure 5: Vibrational frequencies of endocyclic C=C bonds

The exocyclic double bonds exhibit an increase in frequency with decrease in ring size. The exocyclic double bond on six-membered ring absorbs at 1651 cm^{-1} and it is shifted to 1780 cm^{-1} in case of exocyclic double bond on cyclopropane. The allenes show the highest double bond absorptions at 1940 cm^{-1}.



1651 cm^{-1} 1657 cm^{-1} 1678 cm^{-1} 1780 cm^{-1}

Figure 6: Vibrational frequencies of exocyclic C=C bonds

Six-membered rings with carbonyl group e.g. cyclohexanone absorb at normal value i.e. 1715 cm^{-1}. Decrease in ring size increases the C=O stretching frequency. Smaller rings require the use of more p- character to make C-C bonds for the requisite small angles (Figure 6).

7.5 Alkynes

Alkynes contain the C≡C group and three characteristic bands can be present, i.e. ≡C–H stretching, ≡C–H bending and C≡C stretching. As the force constant for a triple bond is greater than that for a double bond. Consequently, whereas a C-C stretching vibrations occur between 1300-800 cm^{-1} and the C=C stretching vibration occur in the region 1700-1500 cm^{-1}, the C triple C vibrations are observed at significantly higher frequencies in the region of 2300 to 2050 cm^{-1}. The terminal alkynes show C-C triple bond stretching vibration at 2140-2050 cm^{-1}, whereas the symmetrical or unsymmetrical internal alkynes show either no band or show a very weak C-C triple bond absorption at 2260-2190 cm^{-1}.

The terminal alkynes show a strong and sharp C-H stretching vibration bands in the region 3310-3200 cm^{-1}. The sharpness of this band prevents form the confusion with other absorptions in this region (NH, OH etc).

The C-H bending vibrations in alkynes occur as a strong broad band in the region 700-600 cm^{-1}. The first overtone of this band appears as a weak broad band near 1375-1225 cm^{-1}.

Therefore the frequency of the absorption of C-H bond is a function of the type of hybridization of the carbon to which hydrogen atom is attached. While moving from sp^{3} to sp^{2} and sp hybridized carbons, the s-character increases and so is the bond strength (force constant of C-H bond and the frequency of absorption (Figure 7,8).

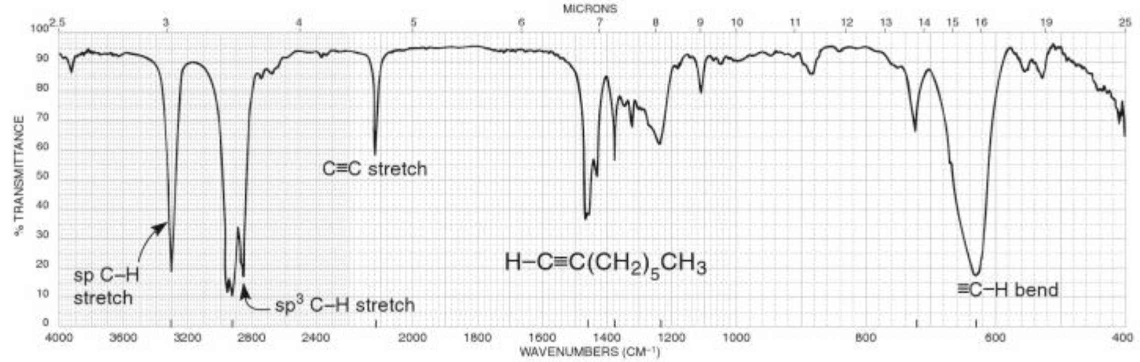


Figure 7: IR-spectrum of 1-octyne

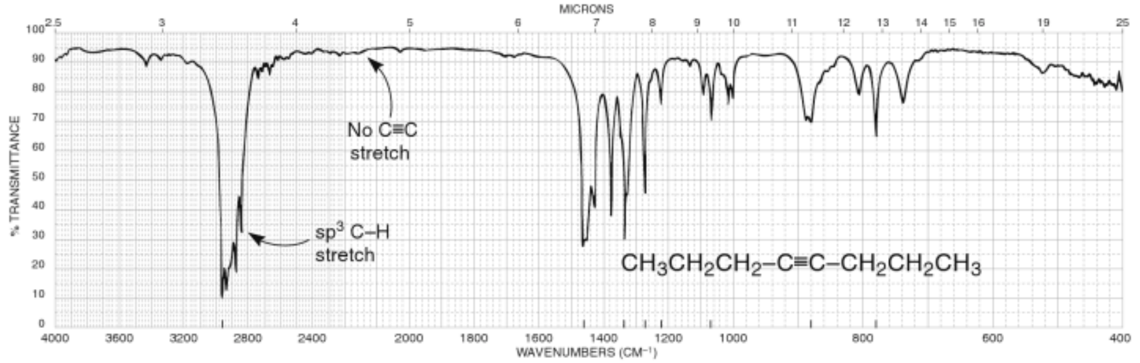


Figure 8: IR-spectrum of 4-octyne

8. Aromatic hydrocarbons

The C–H stretching bands of aromatic compounds appear as a multiple weak bands in the 3100–3000 cm^{-1} range. It is important to note here that the aromatic C–H stretching bands occur at slightly higher frequency (as a shoulder on the stronger alkane C-H stretching bands) than is the C–H stretch in alkanes which appear below 3000 cm^{-1}. Besides the C–H stretch above 3000 cm^{-1}, two other regions of the infrared spectra of aromatic compounds distinguish aromatics from organic compounds that do not have an aromatic ring.

In the region of 2000–1700 cm^{-1}, a series of weak combination and overtone bands appears. However, they are very weak and are observed only in the case of concentrated solutions of highly symmetric benzene derivatives.

The other most prominent bands are in the region of 900-650 cm^{-1} due to the out-of-plane bending of ring C-H bonds. The C–H in-plane bending vibrational bands appear in the regions 1275–1000 cm^{-1}. The bands of the out-of-plane bending vibrations of aromatic compounds are strong and characteristic of the number of hydrogens in the ring, and hence can be used to give the substitution pattern. Mono substituted benzene derivatives exhibit strong absorption bands in the regions 690-710 cm^{-1} and 730-770 cm^{-1}. The absence of band at 690 cm^{-1} indicates the absence of mono substituted phenyl rings in the sample. 1,2-Disubstituted benzenes give one strong absorption band in the region 735-770 cm^{-1} but no band in the region 690-710 cm^{-1}. 1,3-Disubstituted rings give two absorption bands in the region 680-725 cm^{-1} and 750-810 cm^{-1}. 1,4-Disubstituted rings give only one strong absorption band in the region 800-850 cm^{-1}. The IR-spectrum of all the possible di-substituted benzene derivatives are shown below (Figure 9,10, 11,12).

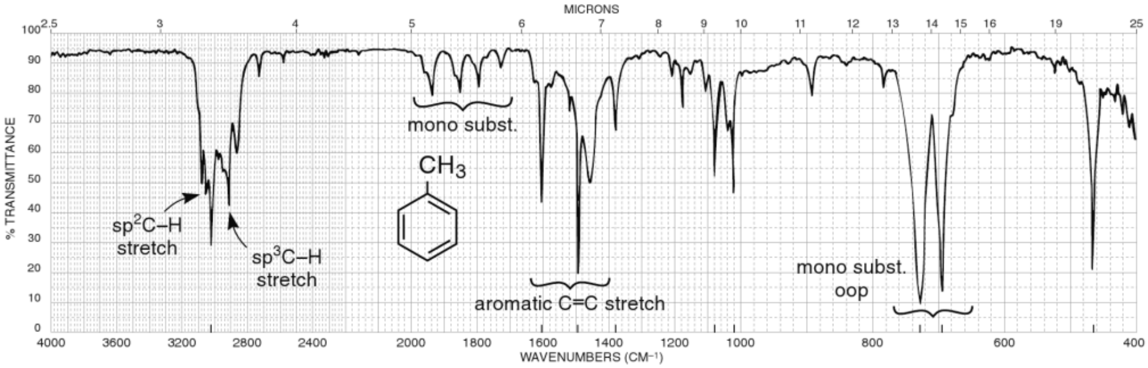


Figure 9: IR-spectrum of toluene

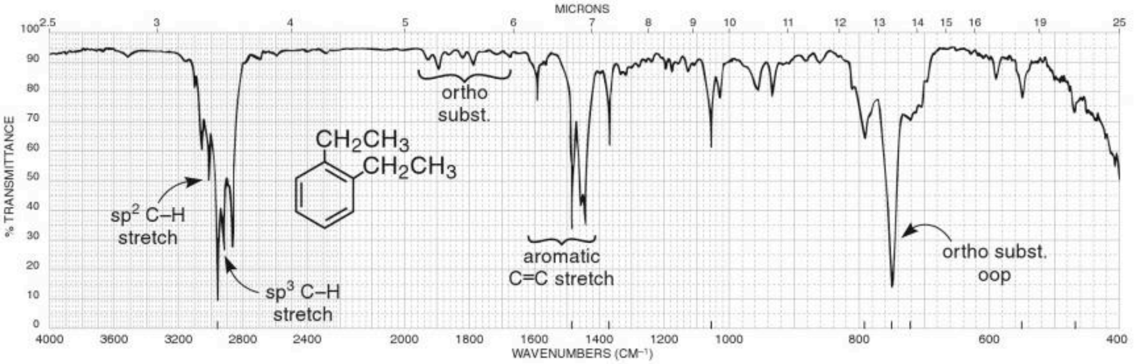


Figure 10: IR-spectrum of 1,2-diethyl benzene

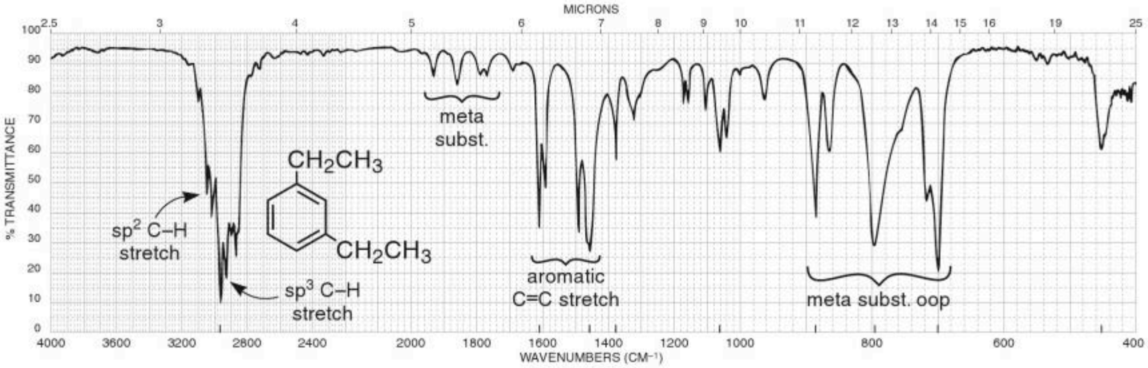


Figure 11: IR-spectrum of 1,3-diethyl benzene

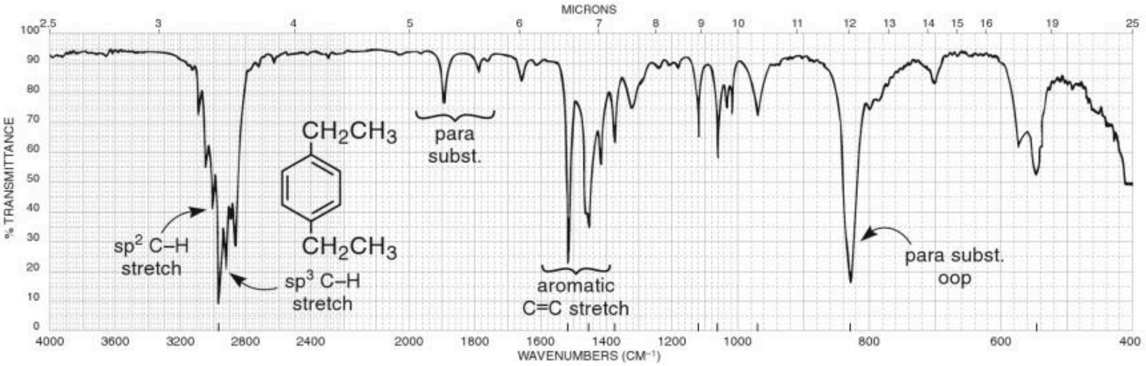


Figure 12: IR-spectrum of 1,4-diethyl benzene

The bands related to other substitution patterns are summarized in the figure given below (Figure 13).

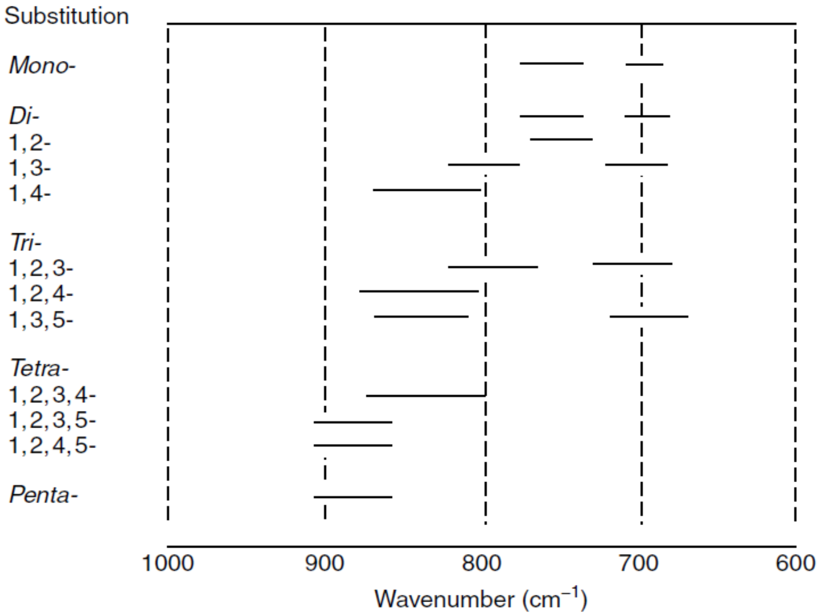


Figure 13: Out-of-plane bending vibrations of ring C-H bonds in substituted aromatic compounds

Aromatic hydrocarbons show absorptions in the regions 1650-1400 cm^{-1} due to C=C stretching vibrations in the aromatic ring. There are normally four bands in this region at about 1600, 1585, 1500 and 1450 cm^{-1} and are due to C=C in-plane vibrations. The absence of these bands indicates that the compound is not aromatic.

9. Summary

1. The stretching frequency of a bond depends on the strength of the bond and the masses of the bonded atoms.
2. Hooke's derived an equation to calculate the approximate vibration frequency of a bond.
3. The vibrational frequency of a bond increases as the number of bonds increases between the two atoms. A C-C triple bond absorbs at higher frequency than a C=C bond followed by a C-C single bond.
4. Hydrogen bonding changes the position and shape of an infrared absorption band. Stronger is the hydrogen bonding, larger are the effects.
5. Ring size and electronic effect such as inductive, resonance also affects the vibrational frequency.
6. Cis-alkenes absorb at higher frequencies and give more intense spectrum than the corresponding trans-alkene.
7. The terminal alkynes show strong C-C triple bond stretching bands while internal alkynes show either no band or show a very weak band due to C-C triple bond.
8. The out of plane bending vibrations for benzene gives important information about the substitution pattern on the benzene ring.