Online Class

SEM-IV (H)

Introduction to IR Spectroscopy

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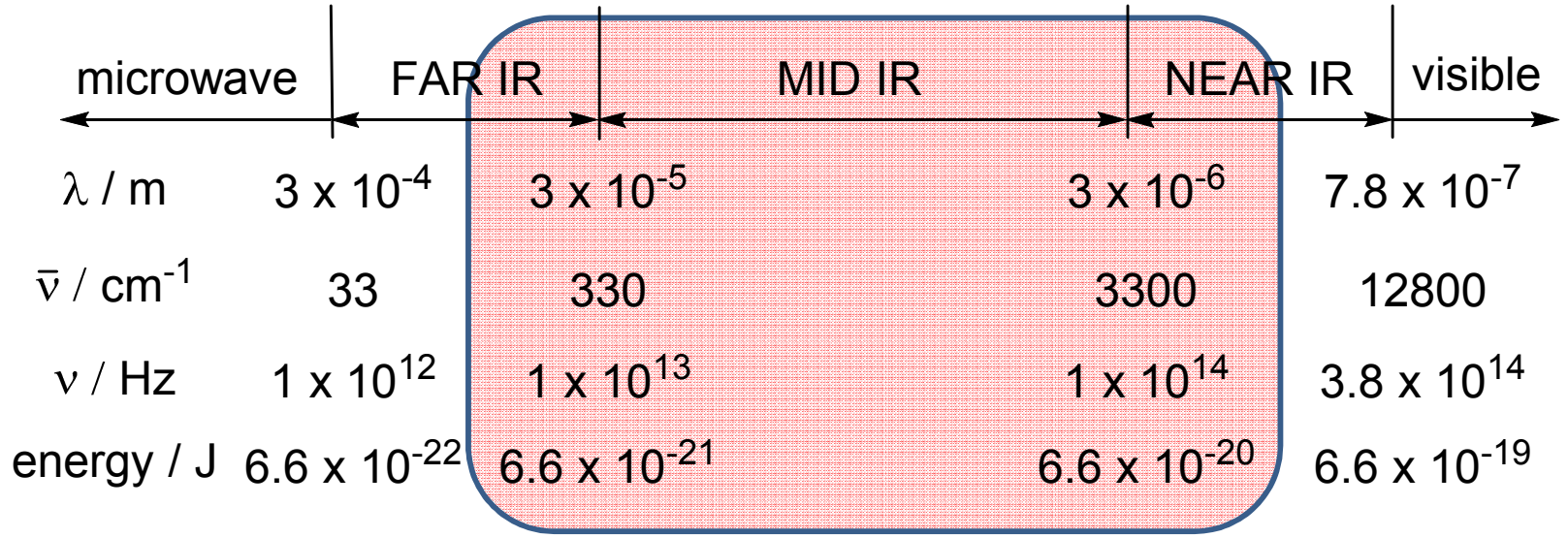
#STAY HOME
#FIGHT CORONA

Infrared spectroscopy deals with transitions within the vibrational levels of a molecule



The region of 4000 – 400 cm^{-1} is of interest to organic chemists as most vibrational transitions of organic functional groups occur in this region

Use of infrared spectrum

Every type of bond in a molecule has a unique natural vibrational frequency. Therefore the IR spectrum of every molecule is unique as much as the finger print of human beings.

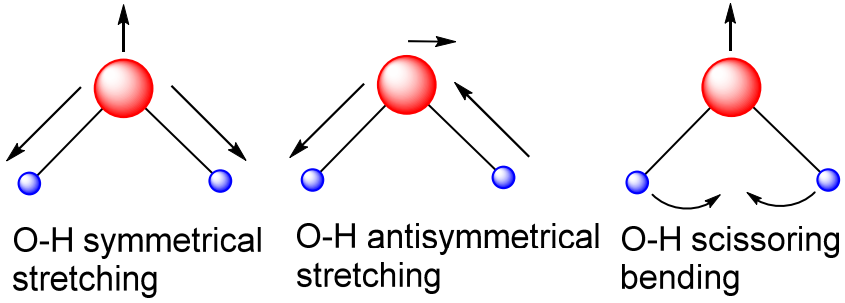
Absorption due to vibrational transitions of each bond type is different and they are confined to a small portion of the IR region.

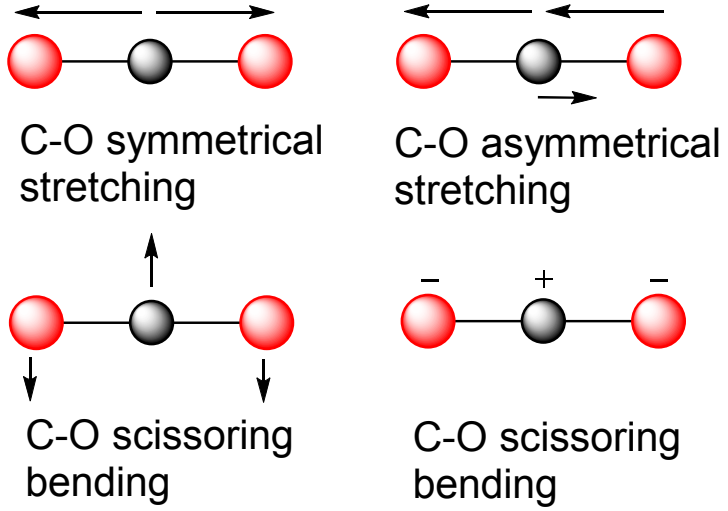
Wave number (cm^{-1})					
4000-2500	2500-2000	2000-1800	1800-1650	1650-1550	1550-650
O-H N-H C-H	C≡C C≡N X=C=Y (C, O, N, S)	Rich information in metal carbonyls (Organo metallics)	Various types of C=O	C=C C=N N=O	C-Cl C-O C-N C-C Finger print region

This allows identification of functional groups in organic molecules because each functional group has a vibrational frequency which appear in a narrow region of the IR region

For a non-linear molecule containing n atoms the number of vibrational degrees of freedom is (3n-6)
For a linear molecule containing n atoms the number of vibrational degrees of freedom is (3n-5)

For example water molecule has 3 degrees of vibrational freedom corresponding to two stretching mode and one bending mode of vibration. These are called fundamental modes or normal modes of vibration and they occur without change of center of gravity of the molecule
For example CO_2 molecule has 4 degrees of vibrational freedom corresponding to two Stretching mode and two bending modes of vibration.

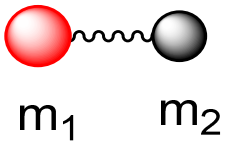




Hook's Law

The vibrational frequencies can be calculated as it relates to bond strength and masses of atoms attached that undergo vibration (Hooke's law)

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



K = force constant, bond order or bond strength and μ is reduced mass

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

From the above equation it is apparent that

(i) stronger the bond higher the vibrational frequency
(ii) higher the masses of atoms lower the vibrational frequency

	C≡C	C=C	C−C
ν_{C-C}	2150	1650	1200 cm^{-1}

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

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

	C≡C−H	C=C−H	C−C−H
ν_{C-H}	3300	3100	2900 cm^{-1}

	C−H	C−H
	3000	1340 cm^{-1}
	stretching	bending

Force constant for bending is smaller than stretching

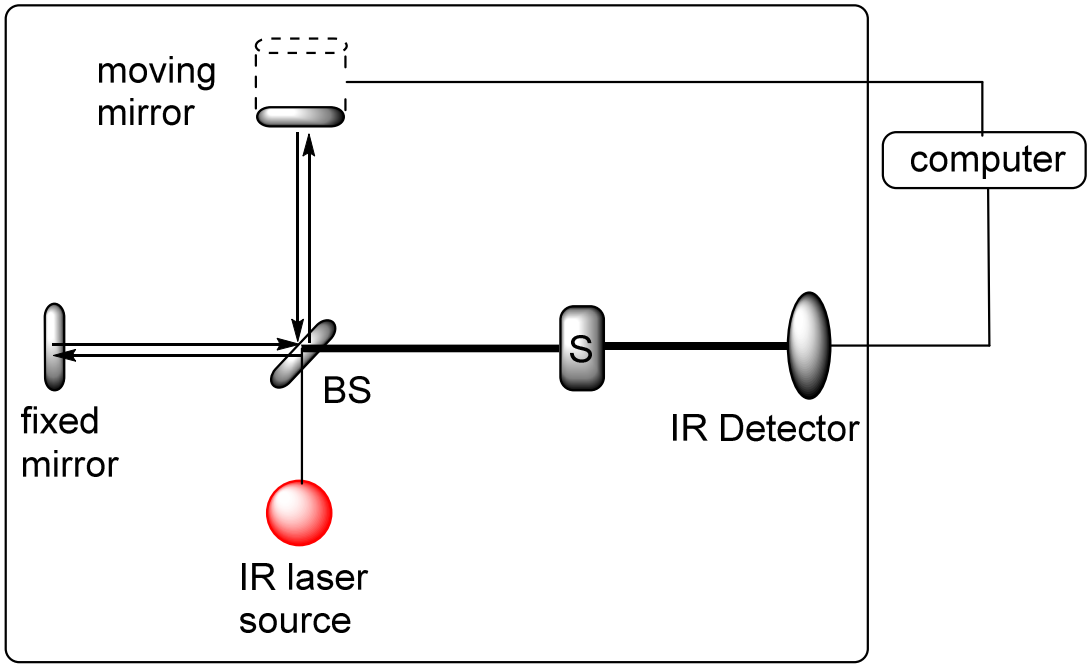
	C−H	C−C	C−O	C−Cl	C−Br	C−I
ν_{C-X}	3000	1200	1100	750	600	500 cm^{-1}

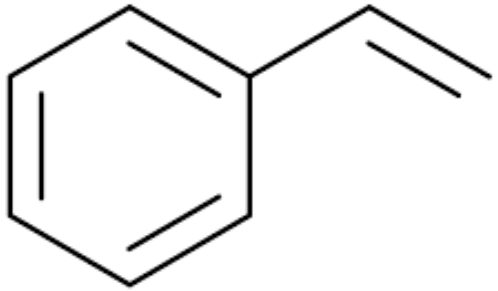
Selection rules for Infrared transitions

- ✓ For a particular vibration to be infrared active there must be a change in the dipole moment of the molecule during the vibration. In other words transition dipole moment must not be zero.
- ✓ Homonuclear diatomic molecules are inactive in the infrared spectrum. They do not have a dipole moment to start with and during the vibration also the dipole moment is zero. eg: H_2, O_2, N_2 etc.
- ✓ Heteronuclear diatomic molecule such as CO, NO are active in IR
- ✓ Symmetrical polyatomic molecules such as CO_2, the symmetric stretching vibration is infrared inactive where as the asymmetric stretching vibration is IR active

$\Delta v = \pm 1$, transition can take place between Adjacent vibrational levels, 0 to 1, 1 to 2 etc.

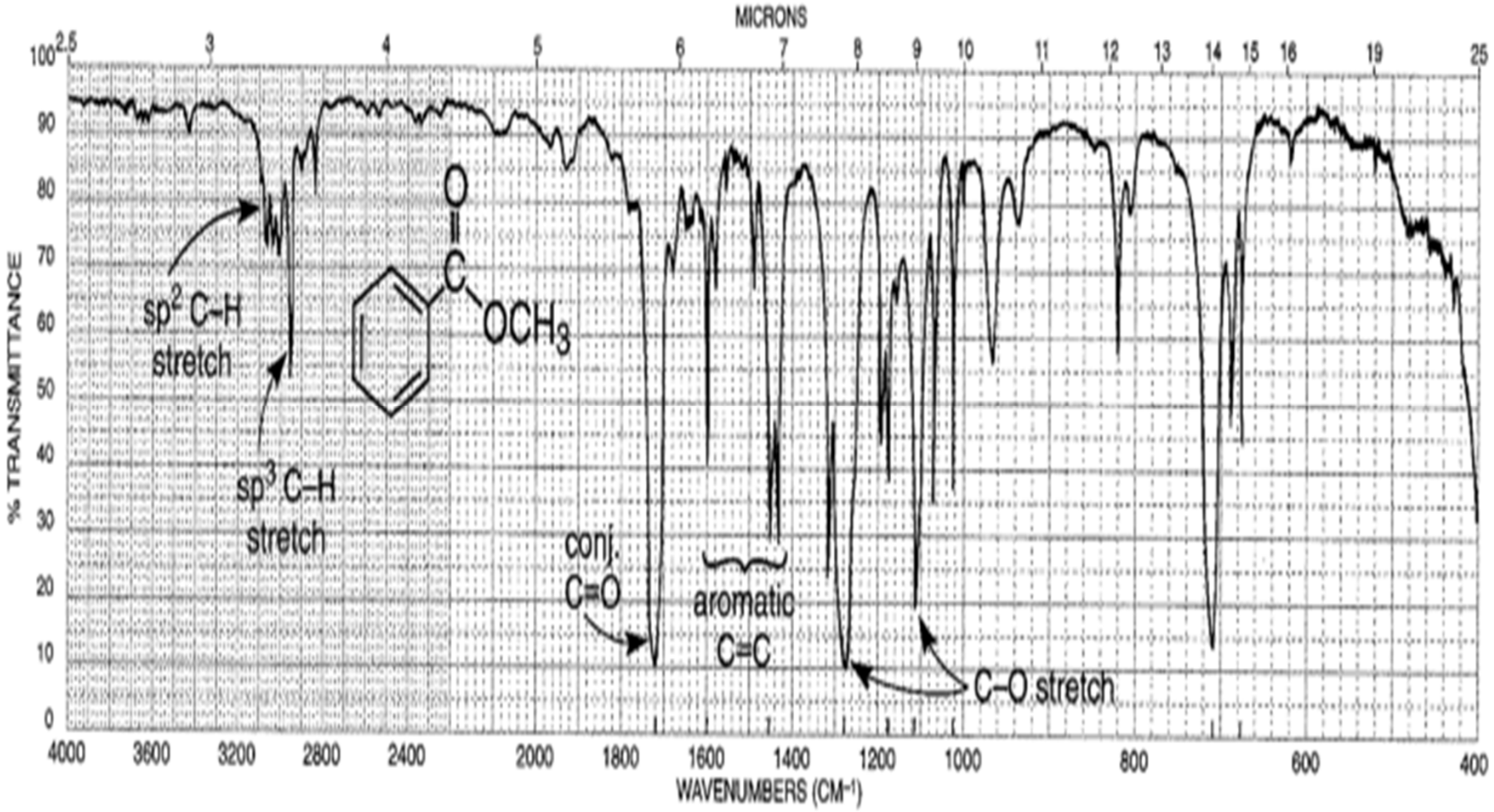
Fourier Transform infrared spectrometer (FTIR)





Calibration of IR spectrum

- ✓ **A thin film of polystyrene is used as a standard for calibration**
- ✓ **Peaks at 1603 and 3062 cm-1 are used to calibrate the spectrum**


MICRONS
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100
90
80
70
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50
40
30
20
10
0
% TRANSMITTANCE
sp2 C–H stretch
sp3 C–H stretch
O
C
OCH3
conj. C=O
aromatic C=C
C–O stretch
4000
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
600
400
WAVENUMBERS (CM-1)

THANK YOU