

UCB008 - APPLIED CHEMISTRY



Infra-red Spectroscopy Series Lecture - V

IR Spectroscopy - Interpretation

by

Prof. Ranjana Prakash

School of Chemistry and Biochemistry

Thapar Institute of Engineering and Technology

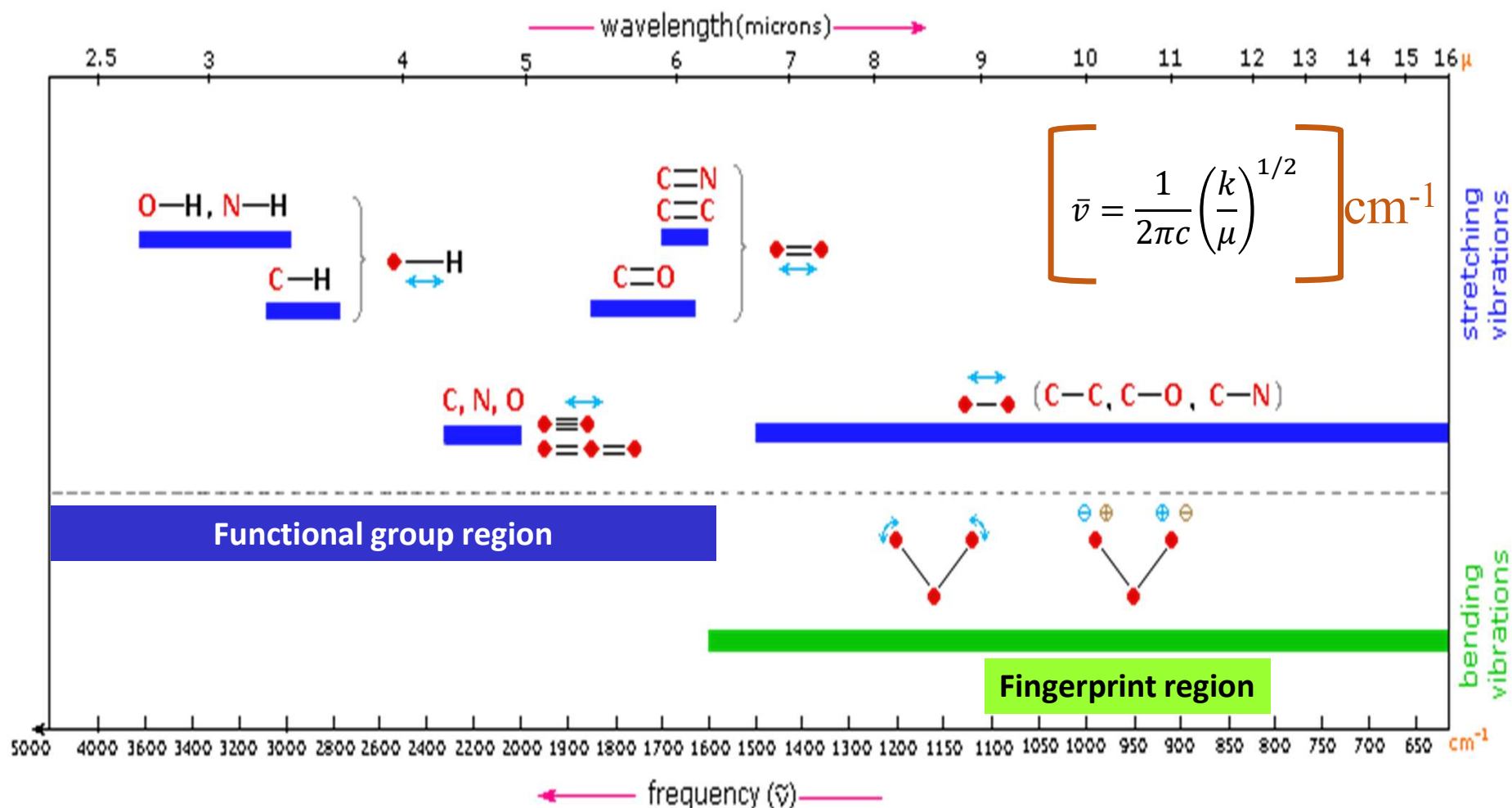
Patiala -147004, India

Learning Outcomes

At the end of this session participants should be able to:

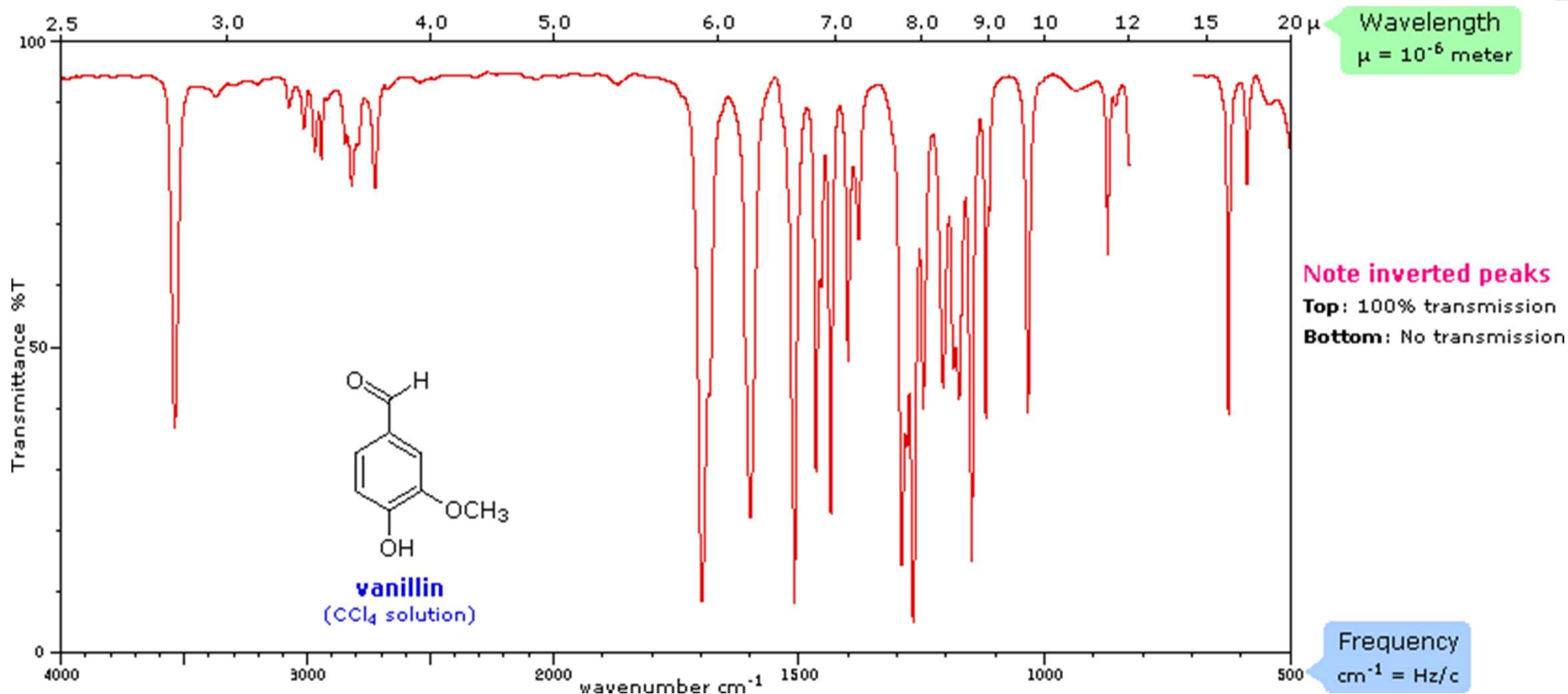
- Interpret an IR spectra

Interpretation of IR spectra



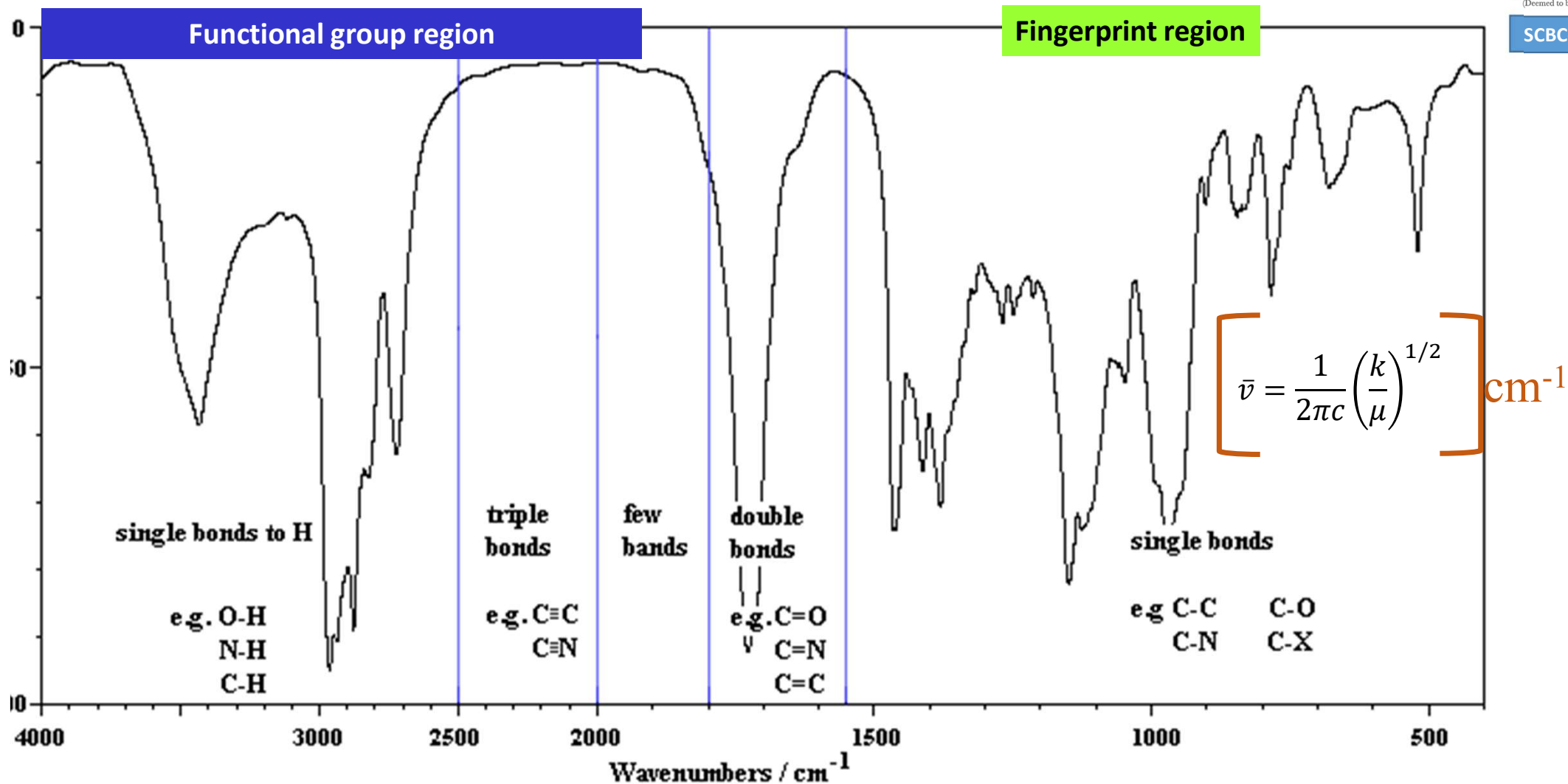
Source: <https://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/Spectrpy/InfraRed/infrared.htm>

Interpretation of IR spectra



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Interpretation of IR spectra

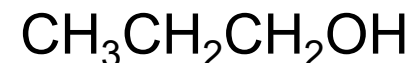
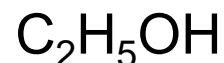
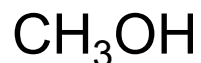


Interpretation of IR spectra

- The complexity of infrared spectra in the 1450 to 600 cm^{-1} region makes it difficult to assign all the absorption bands, and because of the unique patterns found there, it is often called the fingerprint region.
- Absorption bands in the 4000 to 1450 cm^{-1} region are usually due to stretching vibrations of diatomic units, and this is sometimes called the **group frequency** region.
- Group frequency region is also known as **Peak Identification Area** or Functional Group region.

Interpretation of IR spectra

- **For example:**



- If the two samples have same functional group, they show similar absorption above 1450 cm^{-1} , but their spectra will differ in fingerprint region.
- If two samples are giving same spectra in fingerprint region, then they possess same structures or they are enantiomers.

Interpretation of IR spectra

Some General Concepts

- Stretching frequencies are higher than corresponding bending frequencies. (It is easier to bend a bond than to stretch or compress it)
- Triple bonds have higher stretching frequencies than corresponding double bonds, which in turn have higher frequencies than single bonds
- Bonds to hydrogen have higher stretching frequencies than those to heavier atoms
- Since most organic compounds have C-H bonds, a useful rule is that absorption in the 2850 to 3000 cm^{-1} is due to sp^3 C-H stretching; whereas, absorption above 3000 cm^{-1} is from sp^2 C-H stretching or sp C-H stretching if it is near 3300 cm^{-1}

Interpretation of IR spectra

Some General Concepts

- Presence of bands above 1500 cm^{-1} indicates the presence of specific functional group in a compound
- Characteristic wave number of absorption in IR spectra for different groups present in various classes of organic compounds are already been identified and reported in literature
- Group frequency region is also known as Peak Identification Area or Functional Group region.

Interpretation of IR spectra

Carbon-Carbon Bonds

- **Increasing bond order leads to higher frequencies:**
 - C-C 1200 cm^{-1} (fingerprint region)
 - C=C 1600 - 1680 cm^{-1}
 - C \equiv C 2200 cm^{-1}

- **Conjugation lowers the frequency:**
 - isolated C=C 1640-1680 cm^{-1}
 - conjugated C=C 1620-1640 cm^{-1}
 - aromatic C=C approx. 1600 cm^{-1}

- Bonds with more **s** character absorb at a higher frequency.

Interpretation of IR spectra

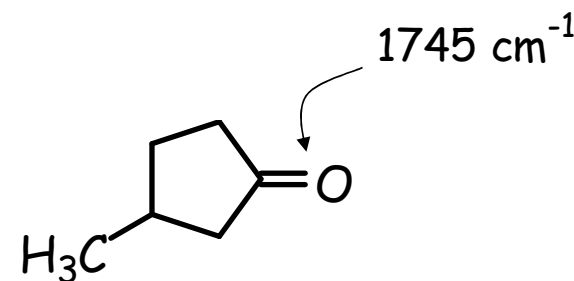
O-H and N-H Bonds

- **Alcohol O-H**
 - broad with rounded tip when hydrogen bonding is present (sharp in the absence of hydrogen bonding)
- **Secondary amine (R_2NH)**
 - Broad (usually) with one sharp spike
- **Primary amine (RNH_2)**
 - Broad (usually) with two sharp spikes.

Interpretation of IR spectra

Carbonyls

- Carbonyl stretches are generally strong:
 - Aldehyde $\sim 1710 \text{ cm}^{-1}$
 - Ketone $\sim 1710 \text{ cm}^{-1}$
 - Carboxylic acid $\sim 1710 \text{ cm}^{-1}$
 - Ester $\sim 1730 - 1740 \text{ cm}^{-1}$
 - Amide $\sim 1640-1680 \text{ cm}^{-1}$
- Conjugation shifts all carbonyls to lower frequencies.
- Ring strain shifts carbonyls to higher frequencies.



Interpretation of IR spectra

Infrared Absorption Frequencies

Functional Group	Range (cm ⁻¹)	Assignment
Alkanes	2850-3000	CH ₃ , CH ₂ & CH 2 or 3 bands
Alkenes	3020-3100 1630-1680 1900-2000	=C-H & =CH ₂ C=C C=C asymmetric stretch
Alkynes	3300 2100-2250	C-H C≡C

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Interpretation of IR spectra

Infrared Absorption Frequencies

Functional Group	Range (cm ⁻¹)	Assignment
Arenes	3030 1600 & 1500	C-H C=C (in ring) (2 bands) (3 if conjugated)
Alcohols & Phenols	3580-3650 3200-3550 970-1250	O-H (free), usually sharp O-H (H-bonded), usually broad C-O
Amines	3400-3500 3300-3400 1000-1250	N-H (1°-amines), 2 bands N-H (2°-amines) C-N
Aldehydes & Ketones	2690-2840(2 bands) 1720-1740 1710-1720 1690 1675 1745 1780	C-H (aldehyde C-H) C=O (saturated aldehyde) C=O (saturated ketone) aryl ketone α, β-unsaturation cyclopentanone cyclobutanone

Interpretation of IR spectra

Infrared Absorption Frequencies

Functional Group	Range (cm ⁻¹)	Assignment
Carboxylic Acids & Derivatives	2500-3300 (acids) overlap C-H	O-H (very broad)
	1705-1720 (acids)	C=O (H-bonded)
	1210-1320 (acids)	O-C
	1785-1815 (acyl halides)	C=O
	1750 & 1820 (anhydrides)	C=O (2-bands)
	1040-1100	O-C
	1735-1750 (esters)	C=O
Nitriles	1000-1300	O-C (2-bands)
	1630-1695 (amides)	C=O (amide one band)
	2240-2260	C≡N (sharp)
Isocyanates, Isothiocyanates, Diimides, Azides & Ketenes	2100-2270	-N=C=O, -N=C=S -N=C=N-, -N ₃ , C=C=O

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In the next session.....

- Applications of IR spectroscopy