Infrared Spectroscopy for Pollution Monitoring
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Lecture-20
IR Spectra Interpretation

So greetings, we will continue our discussion where we had left off regarding the application of IR to a different functional groups. I had shown you this slide in my previous class.

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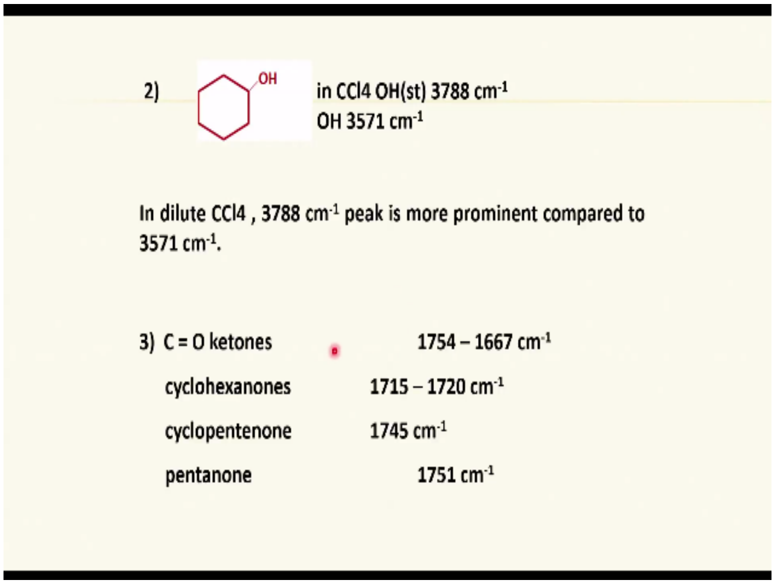

2) in CCl_4 OH(st) 3788 cm^{-1}
OH 3571 cm^{-1}

In dilute CCl_4 , 3788 cm^{-1} peak is more prominent compared to 3571 cm^{-1}.

3) C = O ketones	1754 – 1667 cm^{-1}
cyclohexanones	1715 – 1720 cm^{-1}
cyclopentenone	1745 cm^{-1}
pentanone	1751 cm^{-1}

We were discussing about the peak of carbonyl group that appears between 1715 and 1754 and I had explained to you that irrespective of where the functional compound irrespective of the compound we get the peak of the functional group exactly at the same place. But within the electrical and other stearic effects though you will contribute to shifting the peaks by about 5, 10 centimeter inverse range ok.

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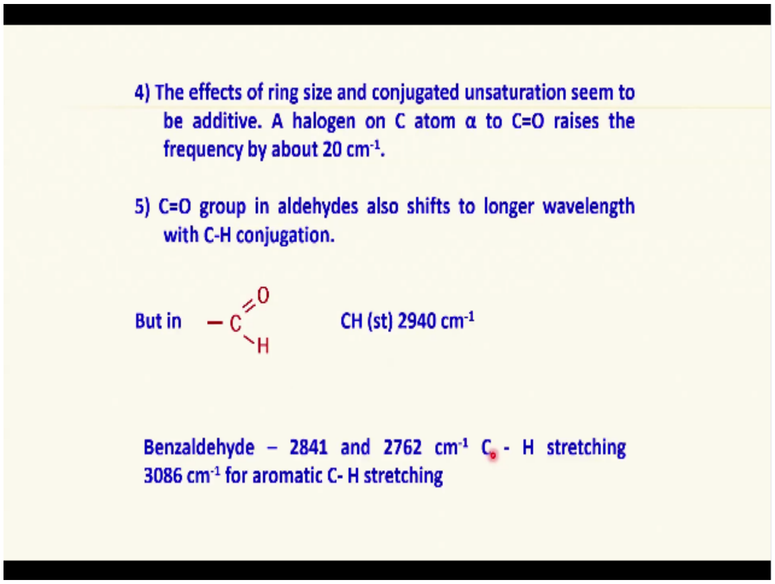

4) The effects of ring size and conjugated unsaturation seem to be additive. A halogen on C atom α to C=O raises the frequency by about 20 cm^{-1}.

5) C=O group in aldehydes also shifts to longer wavelength with C-H conjugation.

But in $-C(=O)H$ CH (st) 2940 cm^{-1}

Benzaldehyde – 2841 and 2762 cm^{-1} C - H stretching
3086 cm^{-1} for aromatic C- H stretching

Now the effects of ring size and the conjugated unsaturation also same to be additive, because I have been talking about the steric effect now. So the ring size and conjugation must be having some effect. So what are the actual effects of such things means they are additive. So halogen and carbon atom alpha2CO raises the frequency by about 20 centimeter, so this is known as keto-enol tautomerism.

You just remember a halogen actually hydrogen and carbon atom alpha to C0 is keto-enol tautomerism, but a halogen on the same alpha carbon atom that is next carbon atom next CO group in a compound. The halogen is normally electron donating group. So it shifts the peak of C0 by about 20 centimeter. So actually halogen I may be wrong but halogen could also be an electron attracting group that is why it raises the frequency.

That means energy it moves to a shorter wavelength by about 20 centimeter, I am wrong but you can correct it and C0 group in aldehydes also shifts to longer wavelength with carbon hydrogen conjugation carbon hydrogen single bond ok. So in this group this COH group aldehyde group, carbon stretching appears at 2940 centimeter inverse ok. So but if it is a take benzaldehyde here also there is carbon hydrogen stretching frequency should off that now.

Because the benzaldehyde also should have carbon and hydrogen in benzene groups, so there it appears at 2841 whereas actual carbon hydrogen stretching frequency here is 2940, so there is about 100 centimeter inverse there is peak in benzaldehyde, but here what I am showing you this stretching frequency attached to carbon hydrogen is 2940, in benzaldehyde what you are seeing is in this 2940 shifts to 2841 ok, that is the stretching frequency attached to this carbon COH group from 2940 to 2841.

And then another frequency is that is in benzaldehyde the benzene group CH group stretching is there. So that appears around 2762 and then there is one more CH stretching frequency 3086 centimeter inverse, this one appear at aromatic stretching. So the same CH stretching will normally give you 3 peaks, so do not get confused if you see so many beaks but they could be one related could be related to benzaldehyde.

And could be the CH in the benzene group, 1 could be the CH in the COH group like that there will be difference and we should be able to identify with experience. But if you look up the database you may suddenly you may see the peaks being assigned specific stretching frequency ok good. So now look let us look at this carboxylic acid anhydride ok, anhydride etc.

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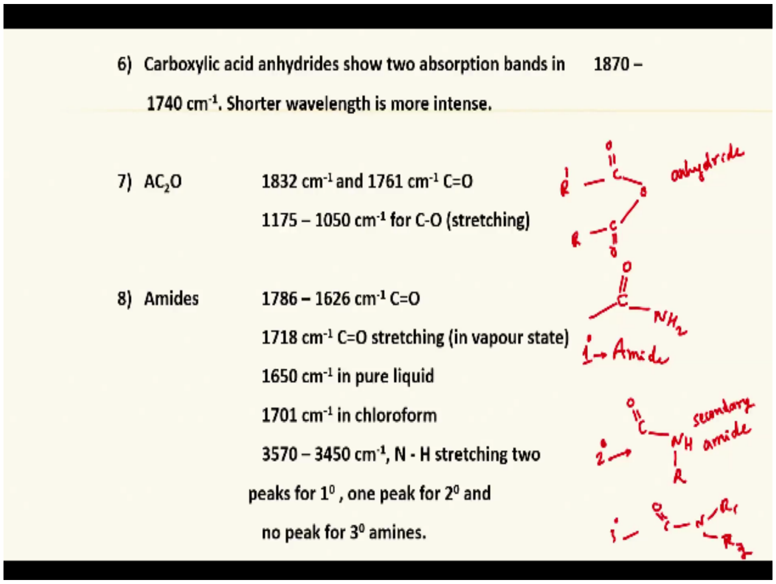
6) Carboxylic acid anhydrides show two absorption bands in 1870 – 1740 cm^{-1}. Shorter wavelength is more intense.

7) AC$_2$O 1832 cm^{-1} and 1761 cm^{-1} C=O
1175 – 1050 cm^{-1} for C-O (stretching)

8) Amides 1786 – 1626 cm^{-1} C=O
1718 cm^{-1} C=O stretching (in vapour state)
1650 cm^{-1} in pure liquid
1701 cm^{-1} in chloroform
3570 – 3450 cm^{-1}, N - H stretching two peaks for 1^0 , one peak for 2^0 and no peak for 3^0 amines.

Acid anhydrides show 2 absorption band that is CO group is already there ok C double bond OCO look at the chemical structure of the anhydrides you will see that there are 2 CO groups that is ketonic groups and again attached with another CO single bond ok. So there are 1780, 1870 to 1740 range you will see 2 absorption peaks ok. But the shorter wavelength peak is the more intensive peak. So if you see 2 peaks and 1 is more intense another is less intense you can definitely say that the compound is anhydride.

Analic anhydride inhalic anhydride succinate anhydride, there are so many anhydrides organic compounds used in different industrial application. So that is another kind of thing, now you look at take a look at the AC2O that is acetic anhydride, acetic anhydride where does it show, it shows 2 peaks 1832 and 1761 centimeter.

And it will also show C-O stretching it should show, so 11 till that stretching frequency of that 1175 to 1050 centimeter inverse for C-O stretching. Now look at amides I have 1786 to 1626, this is assigned C-O 1781 centimeter inverse for C-O stretching, these appears only in vapour state ok. If it is in do you take in a solvent it do not appear and the same beak will appear exactly if you take amide, amide is a liquid.

Suppose amide is a liquid you take it pure liquid it appears at 1650 centimeter, the same beaks shift how they shift depending upon the chemical requirement, chemical environment is variably brought about in this slide. So suppose you take a dissolve amide in chloroform instead of 1650 you will see 1701. So you should not say O that is some other compounds no it is only the steric effect that is showing you all these variations.

But you will see stretching frequencies these cannot change, these are fairly broadband 3570 to 3450 centimeter inverse and then N-H stretching also you should see because there are in amides CO NH2 is the group is not, in amides I have this is an amide ok this is an anhydride, this is an anhydride, so in CO N-H2 we should expect carbon nitrogen is there. So but if it is an amide something like this, this is the secondary amide okay.

This is a secondary amide, if there is no hydrogen inside 2 hydrogen means primary ok. This is secondary amide, tertiary amide means no hydrogen C-O N R1 and R2 this is a tertiary amine. So in tertiary amine again for N-H stretching you will see 2 peaks for corresponding to NH2 group and one peak for secondary and no NH stretching frequency in this thing because they it is connected to carbon atom that is R1 and R2.

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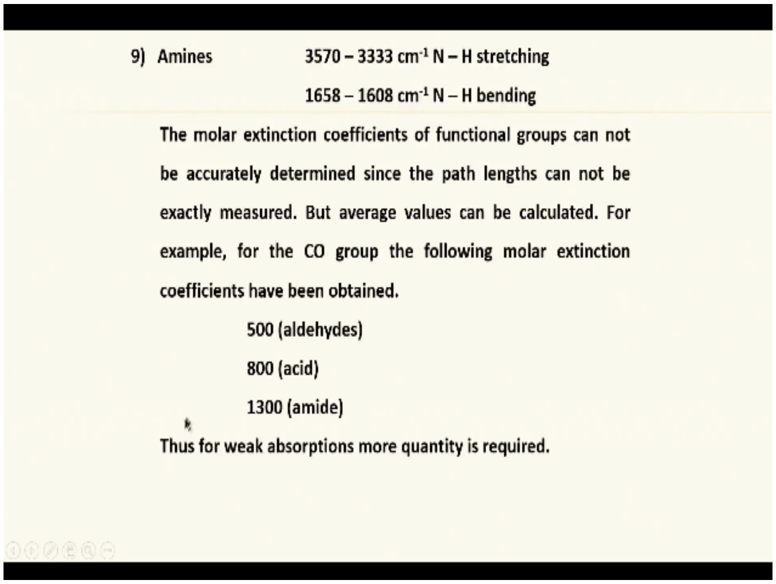

9) Amines 3570 – 3333 cm^{-1} N – H stretching

1658 – 1608 cm^{-1} N – H bending

The molar extinction coefficients of functional groups can not be accurately determined since the path lengths can not be exactly measured. But average values can be calculated. For example, for the CO group the following molar extinction coefficients have been obtained.

500 (aldehydes)

800 (acid)

1300 (amide)

Thus for weak absorptions more quantity is required.

So you can if you know a compound is exactly and amide then pure amide you can say that the weather it is primary, secondary or tertiary by looking at it by at the C-O group as well as N-H stretching frequency. So similarly for amines amine show N-H stretching here and the N-H bending also they will show. But the molar extinction coefficient of functional groups cannot be accurately determined.

Because the sample what we take is very small ok and molar extinction coefficient depends upon the molarity of the substance as well as path length it is Beer-lambert's law that I have taught you in spectrophotometric, it applies everywhere in infrared also. But it is becomes a little compose that is why I i's not used for quantitative analysis as much as in a spectrophotometer. So average values can be calculated of the molar extinction coefficient.

But not be exact values, so for that we need a precise quotes and precise quantity of the substance and then precise measurements of absorption etc. and all transmission for that matter. So but the average values can be calculated. So if you do this the C-O group for the C-O group for aldehydes it is approximately 500, for acid it is approximately 800 and for amides it is approximately 1300.

So for weak absorptions what do you do, if the absorptions is weak, weak means low molar extinction coefficient, small peak just little bit very thing, sometimes the compound is a less in quantity the beak may not appear. So all these positions, all these things one has to consider, so for sometimes our teachers used to say sir I am not getting a peak and no you are taken very small quantity, take double quantity you will see a peak there.

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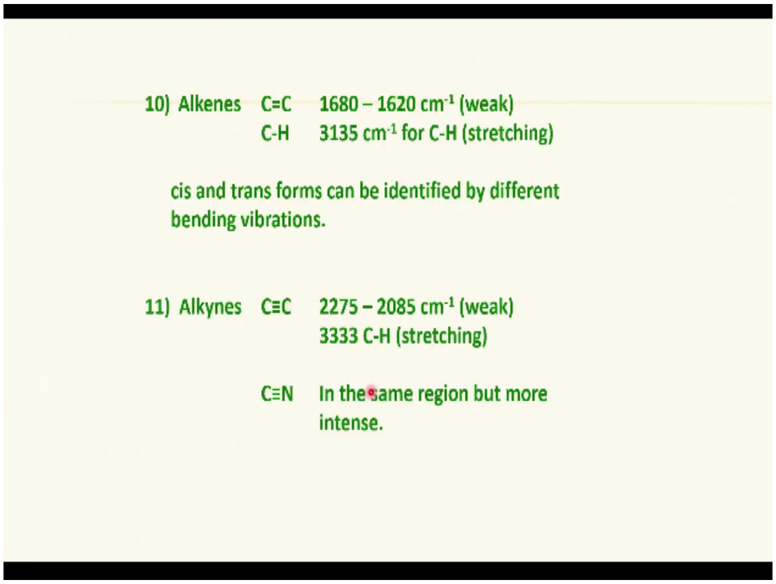

10) Alkenes C=C 1680 – 1620 cm^{-1} (weak)
C-H 3135 cm^{-1} for C-H (stretching)

cis and trans forms can be identified by different
bending vibrations.

11) Alkynes C≡C 2275 – 2085 cm^{-1} (weak)
3333 C-H (stretching)

C≡N In the same region but more
intense.

They were so confident about the appearance of the beaks in IR with respective to functional groups, stretching vibrations and bending vibrations okay. Now alkenes again as usual we expect weak IR spectrum weak beak between 1680 to 1620 and C-H stretching frequency will be strong, that is 3135 centimeter inverse, so in alkenes I can have 2 types one is cis con and another is trans form okay.

So trans form is more symmetrical than the cis form, so they can be identified they will there IR spectrum of bending vibrations will be slightly different and we can identify sis and trans forms of these compounds okay. Alkynes again there is a straight line the compounds that is right compounds they should show weak switching frequency 2275 to 2085 carbon-carbon single bond.

And then here also you can see 3333 this is also stretching frequency but this will be somewhat shaper and carbon nitrogen in the same region of appears but carbon nitrogen is more intense than the carbon-carbon peak. This is nitrile group okay, C=N is nitride and carbon-carbon triple bond is carbon-nitride okay. Then aromatic compounds I can expect C-H stretching and C-H stretching here also.

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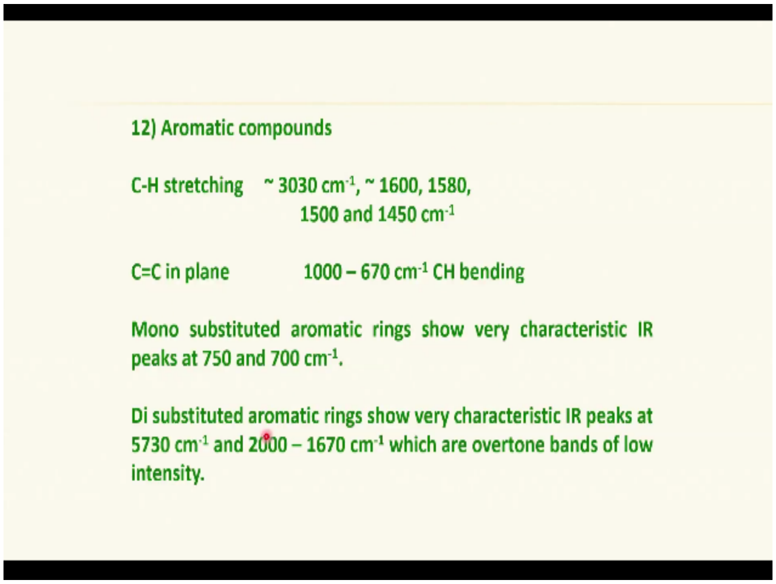

12) Aromatic compounds

C-H stretching ~ 3030 cm^{-1}, ~ 1600, 1580, 1500 and 1450 cm^{-1}

C=C in plane 1000 – 670 cm^{-1} CH bending

Mono substituted aromatic rings show very characteristic IR peaks at 750 and 700 cm^{-1}.

Di substituted aromatic rings show very characteristic IR peaks at 5730 cm^{-1} and 2000 – 1670 cm^{-1} which are overtone bands of low intensity.

And some bending vibrations so 3030, 1600, 1580, 1500 and 1450 centimeter inverse and carbon-carbon double bond we see in plane double bending that appears between 1000 to 670 centimeter inverse you can see that this range is quite large you know it is not a typical of IR. So what it means is it will appear anywhere in this range, peak will be sharp only. So monochromatic aromatic substances that something like 3685 something like okay.

See one nitrogen replacement in a benzene ring that is mono substituted, so they show very characteristic IR peaks between 750 to 700 okay and di substituted C6 H4 something O-H twice or something like that. So such di substituted aromatic compound show very characteristic IR peaks at 5730 centimeter inverse it is quite energetic normal IR range is 4000, so you do not say this in normal IR ok 5738 still towards near IR.

And but there are IR instruments which start from 5000 centimeter inverse, now so 5000 to 5730 centimeter is near IR only. So we will not get a peak here but they do show a peak in that range followed by 2000 to 1670 centimeter inverse which are overtones bands of low intensity ok.

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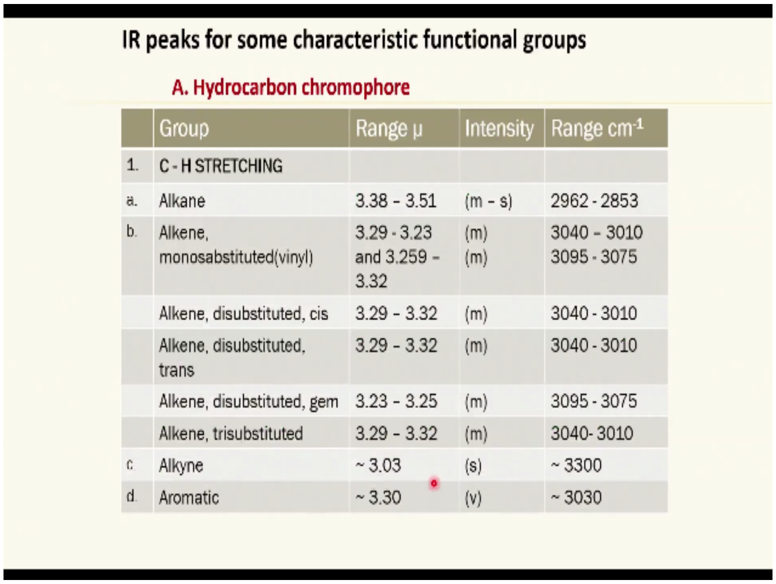

IR peaks for some characteristic functional groups

A. Hydrocarbon chromophore

	Group	Range μ	Intensity	Range cm^{-1}
1.	C - H STRETCHING			
a.	Alkane	3.38 - 3.51	(m - s)	2962 - 2853
b.	Alkene, monosabstituted(vinyl)	3.29 - 3.23 and 3.259 - 3.32	(m) (m)	3040 - 3010 3095 - 3075
	Alkene, disubstituted, cis	3.29 - 3.32	(m)	3040 - 3010
	Alkene, disubstituted, trans	3.29 - 3.32	(m)	3040 - 3010
	Alkene, disubstituted, gem	3.23 - 3.25	(m)	3095 - 3075
	Alkene, trisubstituted	3.29 - 3.32	(m)	3040- 3010
c.	Alkyne	~ 3.03	(s)	~ 3300
d.	Aromatic	~ 3.30	(v)	~ 3030

Now some of these things what I have shown you earlier I am showing you in the form of a table ok this is group, this is the range, this is the intensity and this is range in centimeters inverse, this is microns, so C-H stretching etc. alkane, alkene monosabstituted that is vinyl group etc. and I will not go into more into details, but I am providing you these slides for your convenience okay. So you need not remember this.

But you can use it as a ready reference but this ready reference will help you only in this course rather than in your day-to-day life because in your day today life if you have access to a computer you can have access to data much more complicated and much more detailed accessibility for IR peaks. So we have alkene di substituted cis is 3040, alkene disubstituted trans is 3010 or something like that somewhere in that range ok.

Both are medium intensity bands, so disubstitute gem disubstituted part appearances is here 3095, and 3075, alkene is 3040 to 3010. So alkaline is 3300, aromatic is 3300 you need not buy or study this for the sake of examination but just like this is towards my teaching contribution to you how to understand a table, what are we looking for see.

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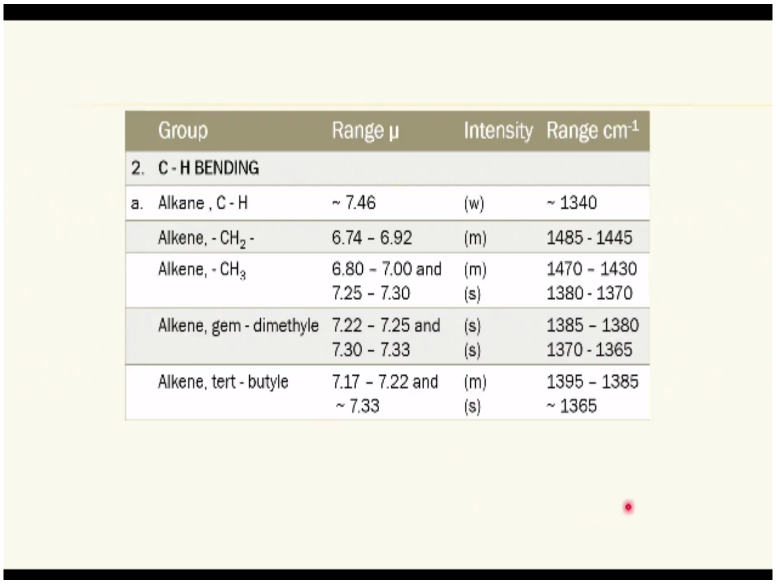

Group	Range μ	Intensity	Range cm^{-1}
2. C - H BENDING			
a. Alkane , C - H	~ 7.46	(w)	~ 1340
Alkene, - CH_2 -	6.74 – 6.92	(m)	1485 - 1445
Alkene, - CH_3	6.80 – 7.00 and 7.25 – 7.30	(m) (s)	1470 – 1430 1380 - 1370
Alkene, gem - dimethyle	7.22 – 7.25 and 7.30 – 7.33	(s) (s)	1385 – 1380 1370 - 1365
Alkene, tert - butyle	7.17 – 7.22 and ~ 7.33	(m) (s)	1395 – 1385 ~ 1365

Otherwise normally people do not know exactly what kind of information people they get from a table. So now I am going to talk about C-H bending. So the top column headings will remain the same alkanes, alkenes, and alkynes gem dimethyl, alkene tertiary butyl and all these things and these are some of the centimeters inverse range, I am more familiar with centimeters inverse rather than micrometers microns ok.

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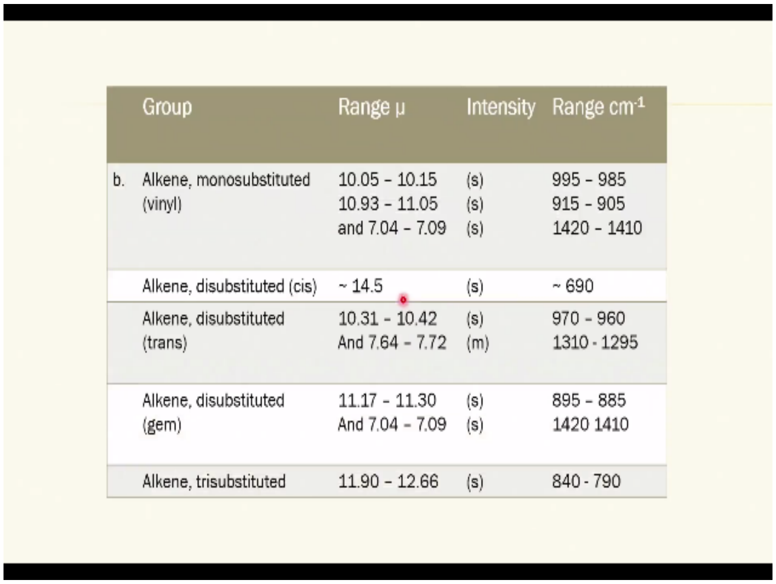

Group	Range μ	Intensity	Range cm^{-1}
b. Alkene, monosubstituted (vinyl)	10.05 – 10.15 10.93 – 11.05 and 7.04 – 7.09	(s) (s) (s)	995 – 985 915 – 905 1420 – 1410
Alkene, disubstituted (cis)	~ 14.5	(s)	~ 690
Alkene, disubstituted (trans)	10.31 – 10.42 And 7.64 – 7.72	(s) (m)	970 – 960 1310 - 1295
Alkene, disubstituted (gem)	11.17 – 11.30 And 7.04 – 7.09	(s) (s)	895 – 885 1420 1410
Alkene, trisubstituted	11.90 – 12.66	(s)	840 - 790

So this is another group alkane disubstituted etc. and here you see them in the low IR range that means these are all bending vibrations ok. The bending vibrations also same to be quite strong the intensity of the peaks also if we study you will know that it is becomes easier for you to identify the peaks.

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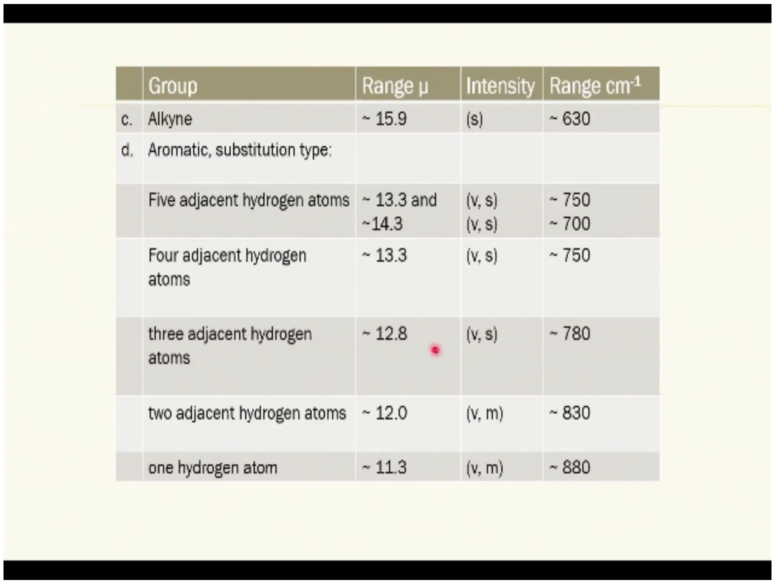

	Group	Range μ	Intensity	Range cm^{-1}
c.	Alkyne	~ 15.9	(s)	~ 630
d.	Aromatic, substitution type:			
	Five adjacent hydrogen atoms	~ 13.3 and ~14.3	(v, s) (v, s)	~ 750 ~ 700
	Four adjacent hydrogen atoms	~ 13.3	(v, s)	~ 750
	three adjacent hydrogen atoms	~ 12.8	(v, s)	~ 780
	two adjacent hydrogen atoms	~ 12.0	(v, m)	~ 830
	one hydrogen atom	~ 11.3	(v, m)	~ 880

Now alkaline, aromatic five adjacent among the aromatic compounds you can see monosabstituted that is 750 to 700 and disubstituted four adjacent hydrogen atoms and that is an auto compound substituted. So that is the 750 three adjacent is 780, two adjacent hydrogen atoms are there 830 like that only one nitrogen and five hydrogen substituted will be somewhere around 880 like that you will see different combinations and possibility for identification as and when you are experience growths okay.

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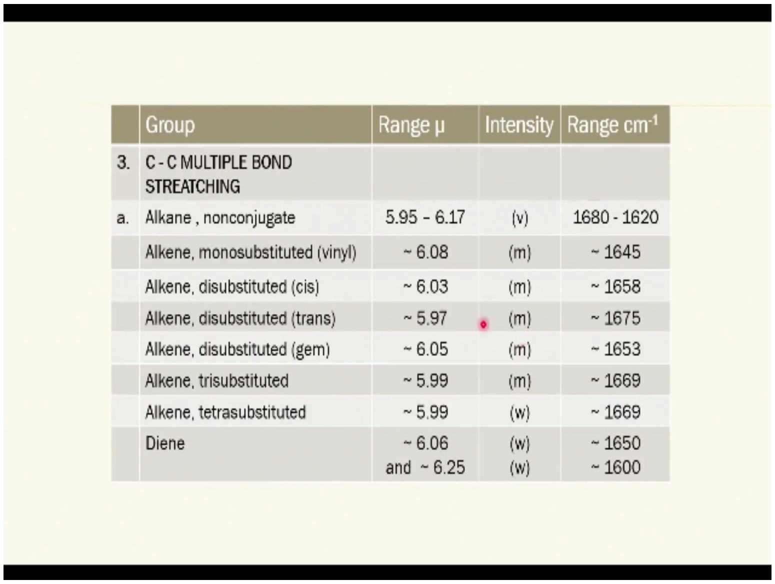

	Group	Range μ	Intensity	Range cm^{-1}
3.	C - C MULTIPLE BOND STREATCHING			
a.	Alkane , nonconjugate	5.95 – 6.17	(v)	1680 - 1620
	Alkene, monosubstituted (vinyl)	~ 6.08	(m)	~ 1645
	Alkene, disubstituted (cis)	~ 6.03	(m)	~ 1658
	Alkene, disubstituted (trans)	~ 5.97	(m)	~ 1675
	Alkene, disubstituted (gem)	~ 6.05	(m)	~ 1653
	Alkene, trisubstituted	~ 5.99	(m)	~ 1669
	Alkene, tetrasubstituted	~ 5.99	(w)	~ 1669
	Diene	~ 6.06 and ~ 6.25	(w) (w)	~ 1650 ~ 1600

So this is carbon-carbon multiple bond stretching, so this is non conjugate alkane around 1680 fingerprint region. So if you do not know a particular compound first thing is go look for the fingerprint region if you can identify aldehyde, ketone etc. etc. well and good. Otherwise you have to go to database disubstituted alkene is somewhere again 1658 all medium this thing and alkene tetra substituted becomes weak.

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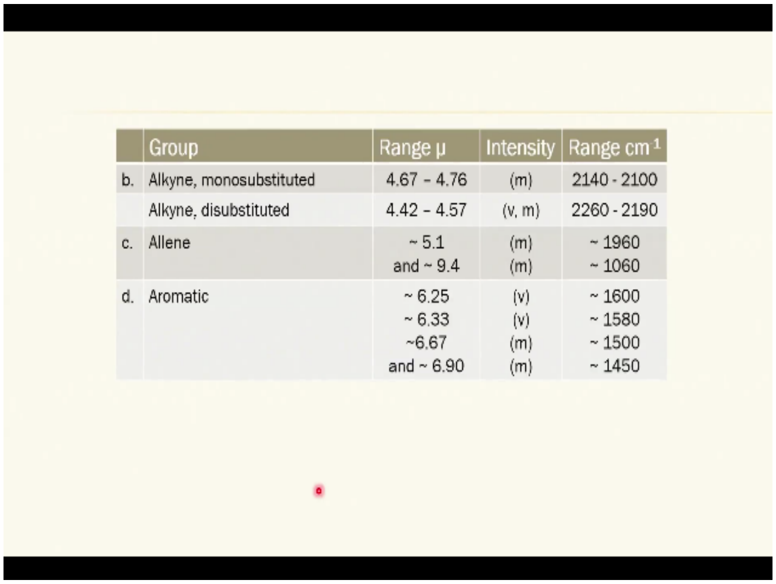

	Group	Range μ	Intensity	Range cm^{-1}
b.	Alkyne, monosubstituted	4.67 – 4.76	(m)	2140 - 2100
	Alkyne, disubstituted	4.42 – 4.57	(v, m)	2260 - 2190
c.	Allene	~ 5.1 and ~ 9.4	(m) (m)	~ 1960 ~ 1060
d.	Aromatic	~ 6.25 ~ 6.33 ~6.67 and ~ 6.90	(v) (v) (m) (m)	~ 1600 ~ 1580 ~ 1500 ~ 1450

But so you will see a small deep in the spectrum not the full peak, so alkynes they have put all of them.

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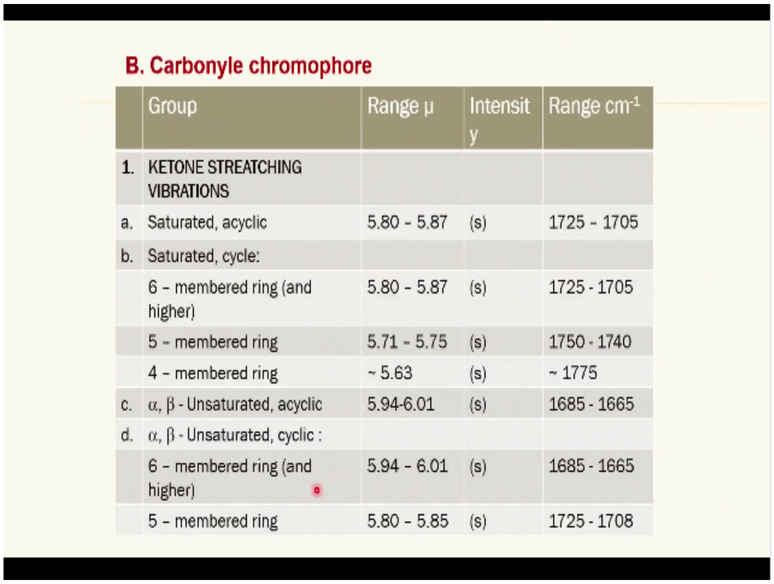

B. Carbonyle chromophore

	Group	Range μ	Intensity	Range cm^{-1}
1.	KETONE STREATCHING VIBRATIONS			
a.	Saturated, acyclic	5.80 – 5.87	(s)	1725 – 1705
b.	Saturated, cycle:			
	6 – membered ring (and higher)	5.80 – 5.87	(s)	1725 - 1705
	5 – membered ring	5.71 – 5.75	(s)	1750 - 1740
	4 – membered ring	~ 5.63	(s)	~ 1775
c.	α, β - Unsaturated, acyclic	5.94-6.01	(s)	1685 - 1665
d.	α, β - Unsaturated, cyclic :			
	6 – membered ring (and higher)	5.94 – 6.01	(s)	1685 - 1665
	5 – membered ring	5.80 – 5.85	(s)	1725 - 1708

Then carbonyl chromophore, I have some of them here ketonic stretching ok that is 1725 saturated cyclic compounds 6 membered ring 1725 to 1705, five membered ring 1740, all of them are within 1680 to 1750. So C-O grouping any person not familiar with IR would also be able to identify C-O groups, if they are there ok. So but a little more experience will help you identify different compound.

For example this last one we will look at it, six membered ring and five membered ring 1685 to 1785 a good organic chemistry this is 6 membered ring because a peak is here like that it is possible to look at different organic compounds and functional groups which I have listed here.

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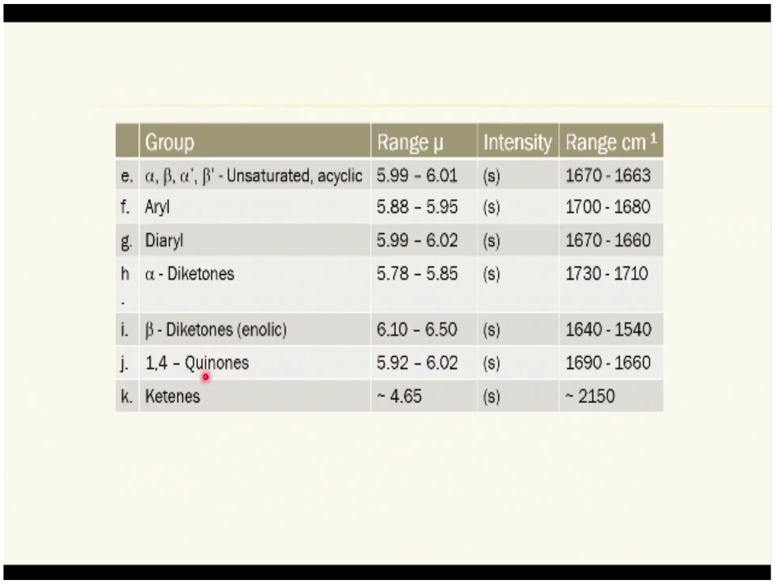

	Group	Range μ	Intensity	Range cm^{-1}
e.	α, β, α', β' - Unsaturated, acyclic	5.99 – 6.01	(s)	1670 - 1663
f.	Aryl	5.88 – 5.95	(s)	1700 - 1680
g.	Diaryl	5.99 – 6.02	(s)	1670 - 1660
h.	α - Diketones	5.78 – 5.85	(s)	1730 - 1710
i.	β - Diketones (enolic)	6.10 – 6.50	(s)	1640 - 1540
j.	1,4 – Quinones	5.92 – 6.02	(s)	1690 - 1660
k.	Ketenes	~ 4.65	(s)	~ 2150

So it should not be a problem for you to work depending upon your requirement.

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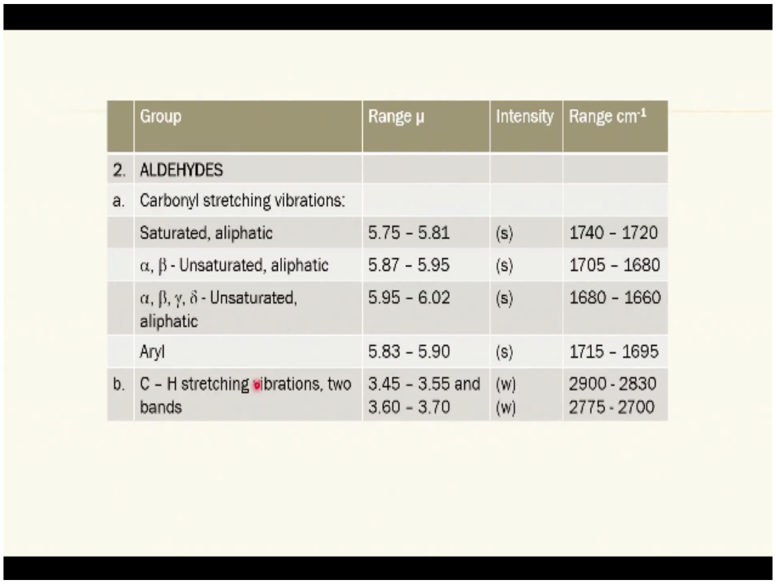

	Group	Range μ	Intensity	Range cm^{-1}
2.	ALDEHYDES			
a.	Carbonyl stretching vibrations:			
	Saturated, aliphatic	5.75 – 5.81	(s)	1740 – 1720
	α, β - Unsaturated, aliphatic	5.87 – 5.95	(s)	1705 – 1680
	α, β, γ, δ - Unsaturated, aliphatic	5.95 – 6.02	(s)	1680 – 1660
	Aryl	5.83 – 5.90	(s)	1715 – 1695
b.	C – H stretching vibrations, two bands	3.45 – 3.55 and 3.60 – 3.70	(w) (w)	2900 - 2830 2775 - 2700

Then I have also listed a few other organic compounds aldehydes, ketones etc. I am not going into details, but it is only for the completeness of the teaching programme ok.

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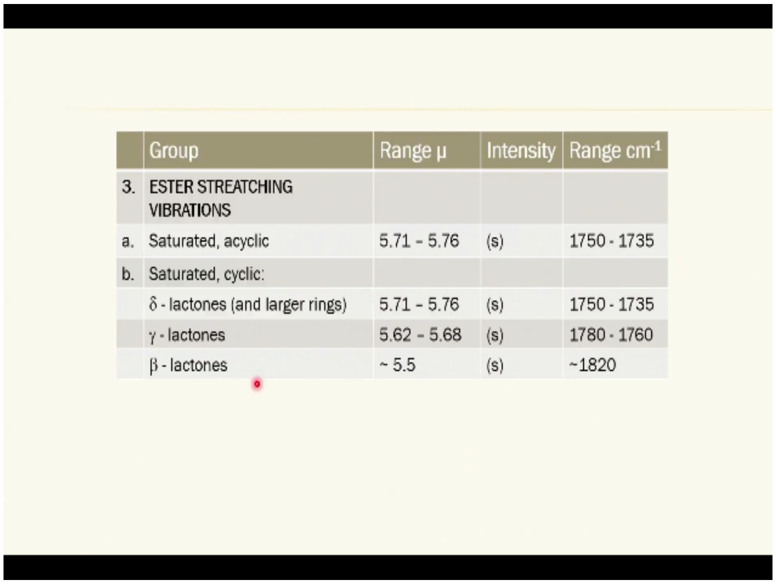

	Group	Range μ	Intensity	Range cm⁻¹
3.	ESTER STREATCHING VIBRATIONS			
a.	Saturated, acyclic	5.71 – 5.76	(s)	1750 - 1735
b.	Saturated, cyclic:			
	δ - lactones (and larger rings)	5.71 – 5.76	(s)	1750 - 1735
	γ - lactones	5.62 – 5.68	(s)	1780 - 1760
	β - lactones	~ 5.5	(s)	~1820

Ester streatching I have given you here, some of the electrons are there.

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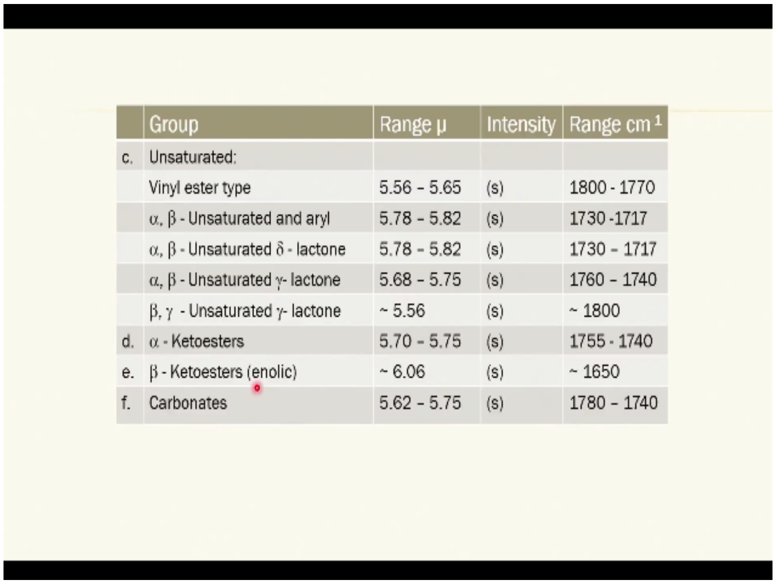

	Group	Range μ	Intensity	Range cm⁻¹
c.	Unsaturated:			
	Vinyl ester type	5.56 – 5.65	(s)	1800 - 1770
	α, β - Unsaturated and aryl	5.78 – 5.82	(s)	1730 -1717
	α, β - Unsaturated δ - lactone	5.78 – 5.82	(s)	1730 – 1717
	α, β - Unsaturated γ- lactone	5.68 – 5.75	(s)	1760 – 1740
	β, γ - Unsaturated γ- lactone	~ 5.56	(s)	~ 1800
d.	α - Ketoesters	5.70 – 5.75	(s)	1755 - 1740
e.	β - Ketoesters (enolic)	~ 6.06	(s)	~ 1650
f.	Carbonates	5.62 – 5.75	(s)	1780 – 1740

Electrons are useful for milk and milky products ok, so keta esters they are all fragrances and carboxylic acids again it is quite possible to identify several carboxylic acid because of the presence of C-O bond carbonyl group.

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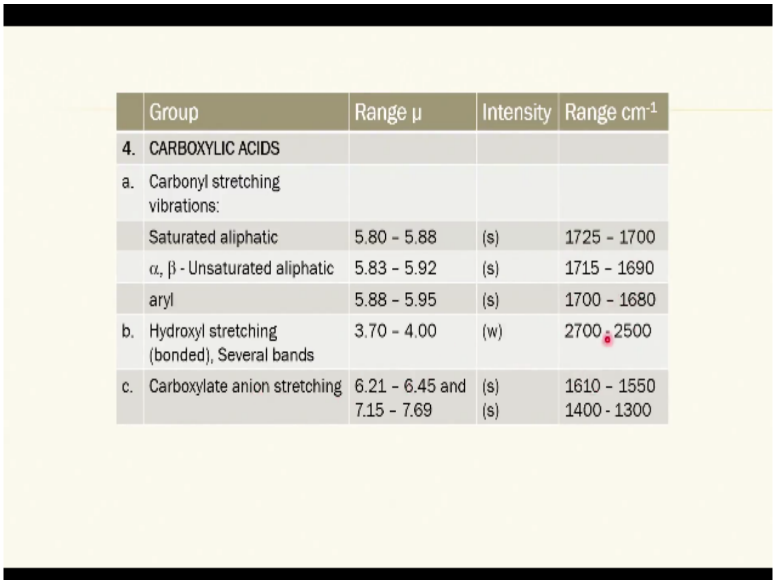

	Group	Range μ	Intensity	Range cm^{-1}
4.	CARBOXYLIC ACIDS			
a.	Carbonyl stretching vibrations:			
	Saturated aliphatic	5.80 - 5.88	(s)	1725 - 1700
	α, β - Unsaturated aliphatic	5.83 - 5.92	(s)	1715 - 1690
	aryl	5.88 - 5.95	(s)	1700 - 1680
b.	Hydroxyl stretching (bonded), Several bands	3.70 - 4.00	(w)	2700 - 2500
c.	Carboxylate anion stretching	6.21 - 6.45 and 7.15 - 7.69	(s) (s)	1610 - 1550 1400 - 1300

And then followed by a stretching and dynamic stretching and all those things are there, so some of these things are there.

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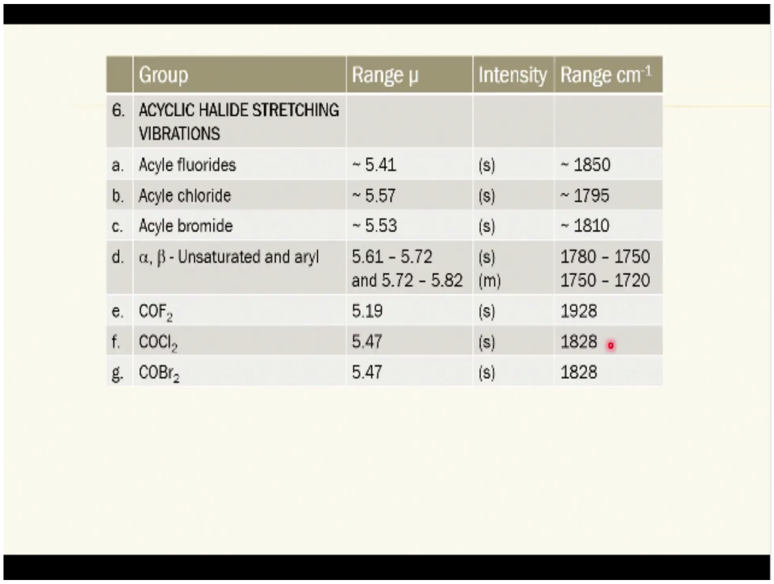

	Group	Range μ	Intensity	Range cm^{-1}
6.	ACYCLIC HALIDE STRETCHING VIBRATIONS			
a.	Acyle fluorides	~ 5.41	(s)	~ 1850
b.	Acyle chloride	~ 5.57	(s)	~ 1795
c.	Acyle bromide	~ 5.53	(s)	~ 1810
d.	α, β - Unsaturated and aryl	5.61 - 5.72 and 5.72 - 5.82	(s) (m)	1780 - 1750 1750 - 1720
e.	COF_2	5.19	(s)	1928
f.	$COCl_2$	5.47	(s)	1828
g.	$COBr_2$	5.47	(s)	1828

You can identify compounds like fluorine, chlorine and bromine depending upon just look at these things 1928, 1828 centimeter inverse and 1828. So most of the alicyclic halide stretching frequencies with fluoride, chloride, bromide they can be easily identified without chemical analysis ok.

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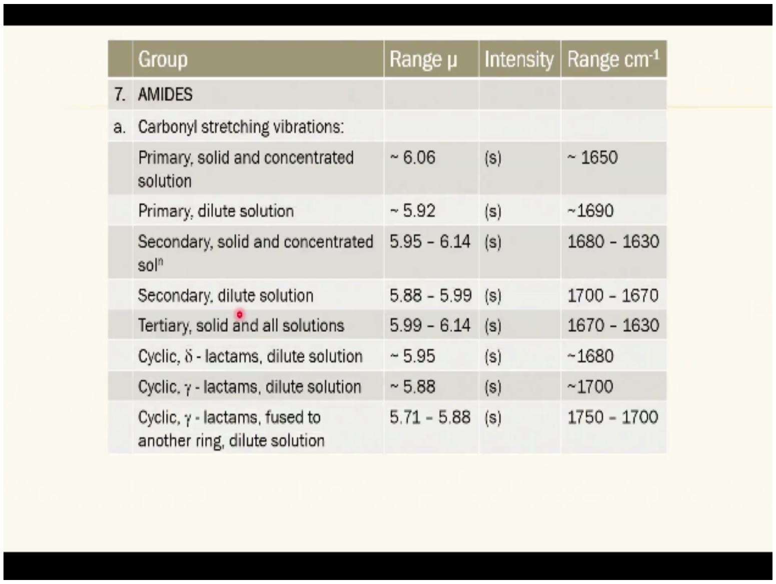

	Group	Range μ	Intensity	Range cm^{-1}
7.	AMIDES			
a.	Carbonyl stretching vibrations:			
	Primary, solid and concentrated solution	~ 6.06	(s)	~ 1650
	Primary, dilute solution	~ 5.92	(s)	~1690
	Secondary, solid and concentrated sol^{n}	5.95 - 6.14	(s)	1680 - 1630
	Secondary, dilute solution	5.88 - 5.99	(s)	1700 - 1670
	Tertiary, solid and all solutions	5.99 - 6.14	(s)	1670 - 1630
	Cyclic, δ - lactams, dilute solution	~ 5.95	(s)	~1680
	Cyclic, γ - lactams, dilute solution	~ 5.88	(s)	~1700
	Cyclic, γ - lactams, fused to another ring, dilute solution	5.71 - 5.88	(s)	1750 - 1700

So amides again I have primary, secondary, tertiary dilute solution, solids and all solutions and like that one can look at it I will not go into details of the number, but suffice it to say that you can have many organic compounds like this is a cyclic compounds, beta lactam, urease, urethane, imides.

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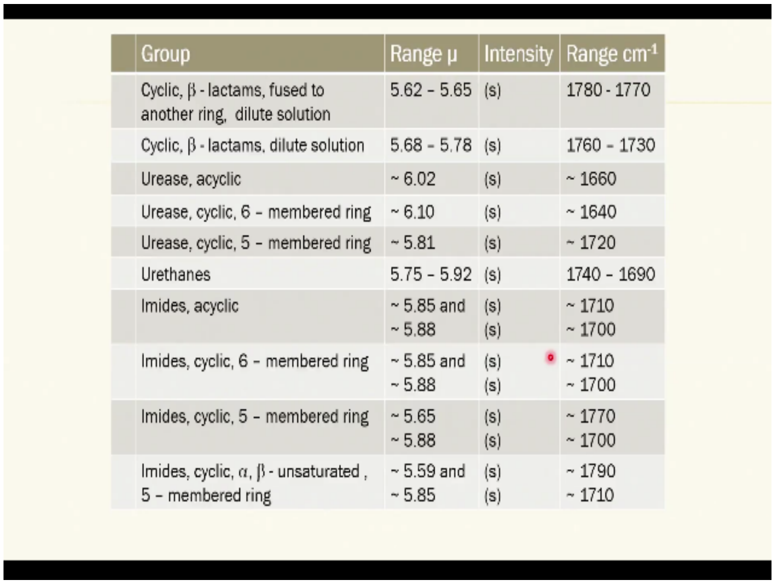

Group	Range μ	Intensity	Range cm^{-1}
Cyclic, β - lactams, fused to another ring, dilute solution	5.62 - 5.65	(s)	1780 - 1770
Cyclic, β - lactams, dilute solution	5.68 - 5.78	(s)	1760 - 1730
Urease, acyclic	~ 6.02	(s)	~ 1660
Urease, cyclic, 6 - membered ring	~ 6.10	(s)	~ 1640
Urease, cyclic, 5 - membered ring	~ 5.81	(s)	~ 1720
Urethanes	5.75 - 5.92	(s)	1740 - 1690
Imides, acyclic	~ 5.85 and ~ 5.88	(s) (s)	~ 1710 ~ 1700
Imides, cyclic, 6 - membered ring	~ 5.85 and ~ 5.88	(s) (s)	~ 1710 ~ 1700
Imides, cyclic, 5 - membered ring	~ 5.65 ~ 5.88	(s) (s)	~ 1770 ~ 1700
Imides, cyclic, α, β - unsaturated , 5 - membered ring	~ 5.59 and ~ 5.85	(s) (s)	~ 1790 ~ 1710

All these things can be easily identified using IR ok.

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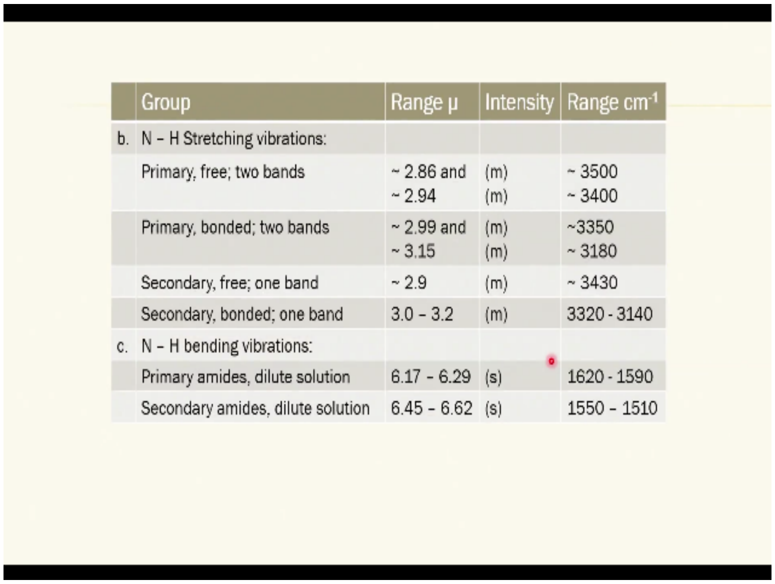

	Group	Range μ	Intensity	Range cm^{-1}
b.	N – H Stretching vibrations:			
	Primary, free; two bands	~ 2.86 and ~ 2.94	(m) (m)	~ 3500 ~ 3400
	Primary, bonded; two bands	~ 2.99 and ~ 3.15	(m) (m)	~3350 ~ 3180
	Secondary, free; one band	~ 2.9	(m)	~ 3430
	Secondary, bonded; one band	3.0 – 3.2	(m)	3320 - 3140
c.	N – H bending vibrations:			
	Primary amides, dilute solution	6.17 – 6.29	(s)	1620 - 1590
	Secondary amides, dilute solution	6.45 – 6.62	(s)	1550 – 1510

This is miscellaneous chromophoric groups O-H stretching hydrogen bonding all this things we can see in IR, but we need more time and more experience or exposure to IR spectrometer ok.

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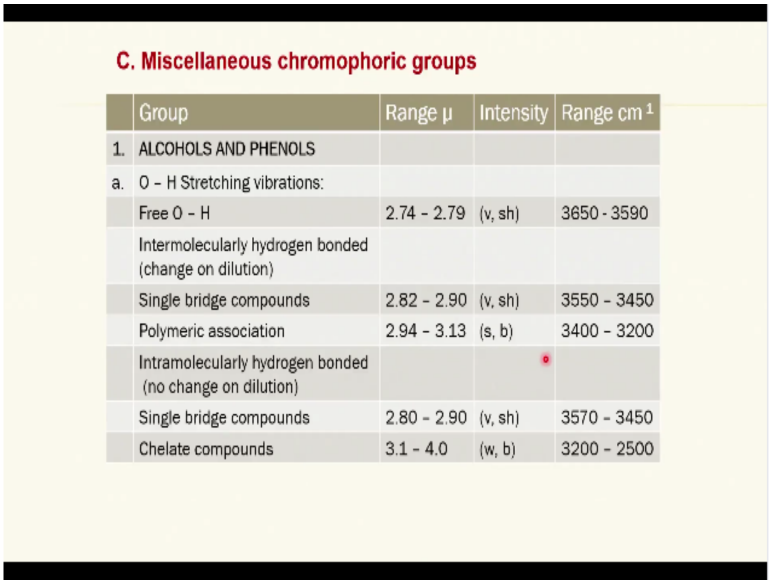

C. Miscellaneous chromophoric groups

	Group	Range μ	Intensity	Range cm^{-1}
1.	ALCOHOLS AND PHENOLS			
a.	O – H Stretching vibrations:			
	Free O – H	2.74 – 2.79	(v, sh)	3650 - 3590
	Intermolecularly hydrogen bonded (change on dilution)			
	Single bridge compounds	2.82 – 2.90	(v, sh)	3550 – 3450
	Polymeric association	2.94 – 3.13	(s, b)	3400 – 3200
	Intramolecularly hydrogen bonded (no change on dilution)			
	Single bridge compounds	2.80 – 2.90	(v, sh)	3570 – 3450
	Chelate compounds	3.1 – 4.0	(w, b)	3200 – 2500

This is O-H bending and C-O stretching for vibrations.

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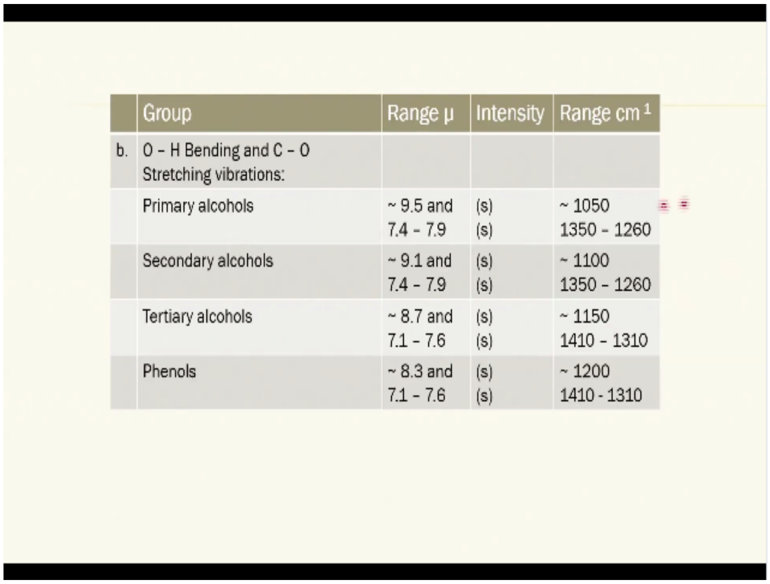

	Group	Range μ	Intensity	Range cm ¹
b.	O – H Bending and C – O Stretching vibrations:			
	Primary alcohols	~ 9.5 and 7.4 – 7.9	(s) (s)	~ 1050 1350 – 1260
	Secondary alcohols	~ 9.1 and 7.4 – 7.9	(s) (s)	~ 1100 1350 – 1260
	Tertiary alcohols	~ 8.7 and 7.1 – 7.6	(s) (s)	~ 1150 1410 – 1310
	Phenols	~ 8.3 and 7.1 – 7.6	(s) (s)	~ 1200 1410 - 1310

Again they are all in the fingerprint range 1400 to 1900 thing 900 range.

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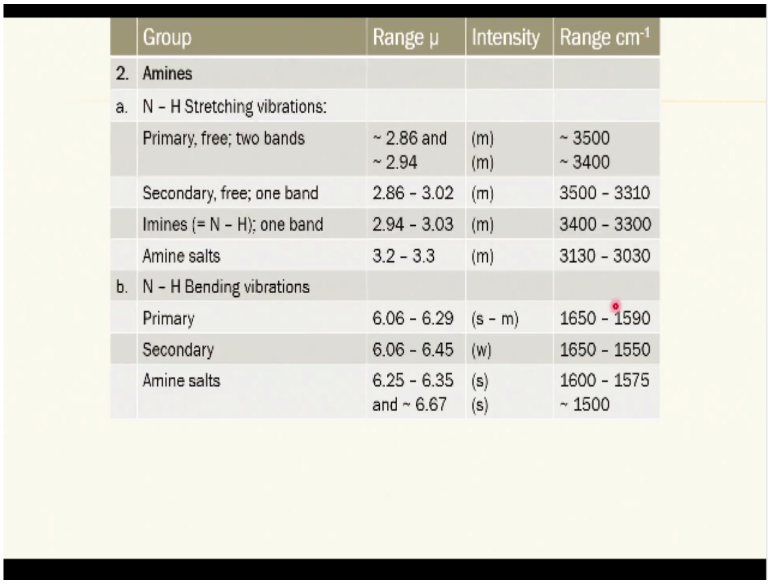

	Group	Range μ	Intensity	Range cm⁻¹
2.	Amines			
a.	N – H Stretching vibrations:			
	Primary, free; two bands	~ 2.86 and ~ 2.94	(m) (m)	~ 3500 ~ 3400
	Secondary, free; one band	2.86 – 3.02	(m)	3500 – 3310
	Imines (= N – H); one band	2.94 – 3.03	(m)	3400 – 3300
	Amine salts	3.2 – 3.3	(m)	3130 – 3030
b.	N – H Bending vibrations			
	Primary	6.06 – 6.29	(s – m)	1650 – 1590
	Secondary	6.06 – 6.45	(w)	1650 – 1550
	Amine salts	6.25 – 6.35 and ~ 6.67	(s) (s)	1600 – 1575 ~ 1500

So some of these again amines all primary, secondary, tertiary, again amines will show primary, will show 2 bands secondary will show one band, like that it will come.

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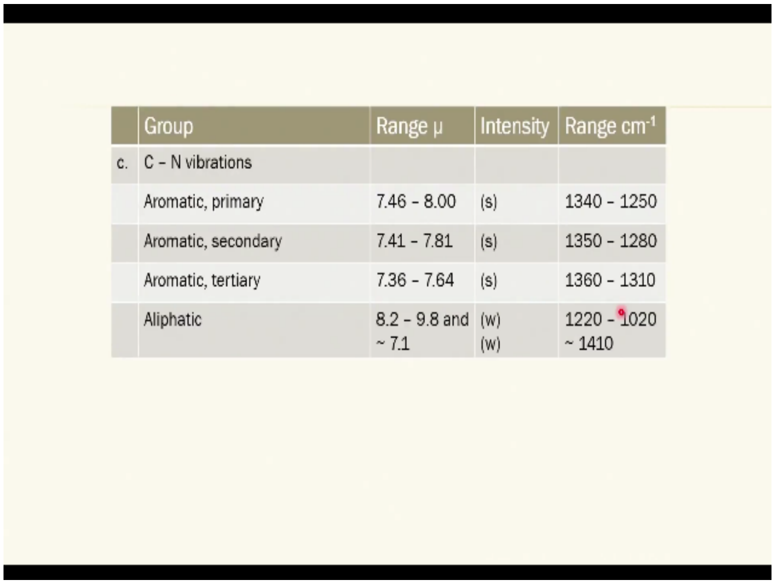

	Group	Range μ	Intensity	Range cm^{-1}
c.	C – N vibrations			
	Aromatic, primary	7.46 – 8.00	(s)	1340 – 1250
	Aromatic, secondary	7.41 – 7.81	(s)	1350 – 1280
	Aromatic, tertiary	7.36 – 7.64	(s)	1360 – 1310
	Aliphatic	8.2 – 9.8 and ~ 7.1	(w) (w)	1220 – 1020 ~ 1410

And then C-N vibrations are there aromatic compounds.

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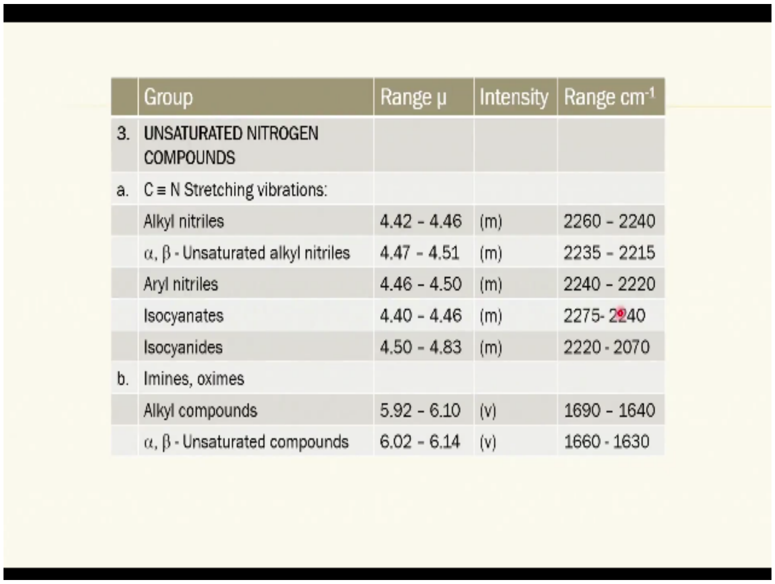

	Group	Range μ	Intensity	Range cm^{-1}
3.	UNSATURATED NITROGEN COMPOUNDS			
a.	C ≡ N Stretching vibrations:			
	Alkyl nitriles	4.42 – 4.46	(m)	2260 – 2240
	α, β - Unsaturated alkyl nitriles	4.47 – 4.51	(m)	2235 – 2215
	Aryl nitriles	4.46 – 4.50	(m)	2240 – 2220
	Isocyanates	4.40 – 4.46	(m)	2275- 2240
	Isocyanides	4.50 – 4.83	(m)	2220 - 2070
b.	Imines, oximes			
	Alkyl compounds	5.92 – 6.10	(v)	1690 – 1640
	α, β - Unsaturated compounds	6.02 – 6.14	(v)	1660 - 1630

Unsaturated organic compounds then nitrates, nitrites, nitrogen compounds they can there also identified.

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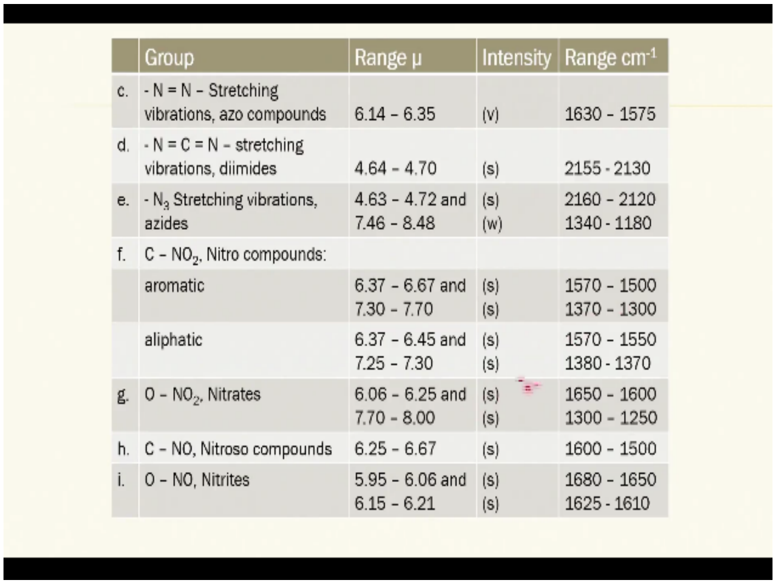
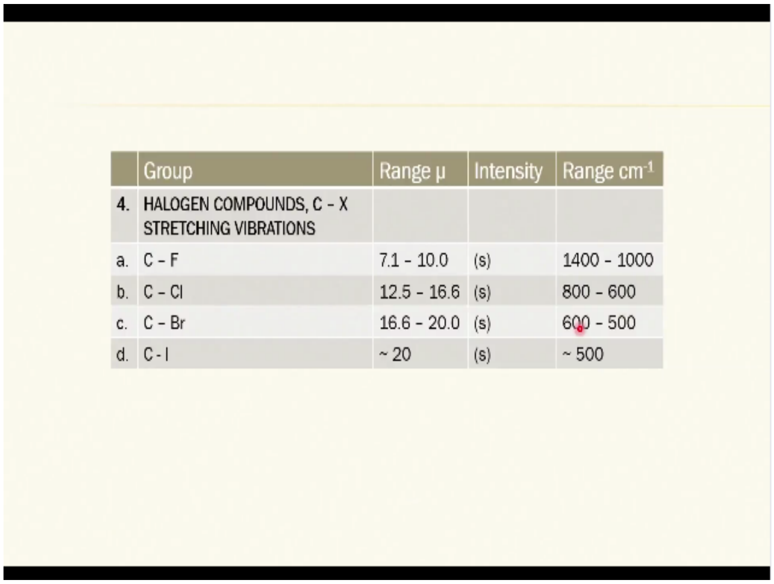


	Group	Range μ	Intensity	Range cm^{-1}
c.	- N = N - Stretching vibrations, azo compounds	6.14 - 6.35	(v)	1630 - 1575
d.	- N = C = N - stretching vibrations, diimides	4.64 - 4.70	(s)	2155 - 2130
e.	- N_3 Stretching vibrations, azides	4.63 - 4.72 and 7.46 - 8.48	(s) (w)	2160 - 2120 1340 - 1180
f.	C - NO_2, Nitro compounds:			
	aromatic	6.37 - 6.67 and 7.30 - 7.70	(s) (s)	1570 - 1500 1370 - 1300
	aliphatic	6.37 - 6.45 and 7.25 - 7.30	(s) (s)	1570 - 1550 1380 - 1370
g.	O - NO_2, Nitrates	6.06 - 6.25 and 7.70 - 8.00	(s) (s)	1650 - 1600 1300 - 1250
h.	C - NO, Nitroso compounds	6.25 - 6.67	(s)	1600 - 1500
i.	O - NO, Nitrites	5.95 - 6.06 and 6.15 - 6.21	(s) (s)	1680 - 1650 1625 - 1610

So what happened is you especially the fingerprint region becomes easier if you know the functional group, if you are handling only one type of organic compound then it will becomes easier for you.

(Refer Slide Time: 25:19)



	Group	Range μ	Intensity	Range cm^{-1}
4.	HALOGEN COMPOUNDS, C - X STRETCHING VIBRATIONS			
a.	C - F	7.1 - 10.0	(s)	1400 - 1000
b.	C - Cl	12.5 - 16.6	(s)	800 - 600
c.	C - Br	16.6 - 20.0	(s)	600 - 500
d.	C - I	~ 20	(s)	~ 500

But if you have an unknown organic compound IR will help you to eliminate many of these substances ok.

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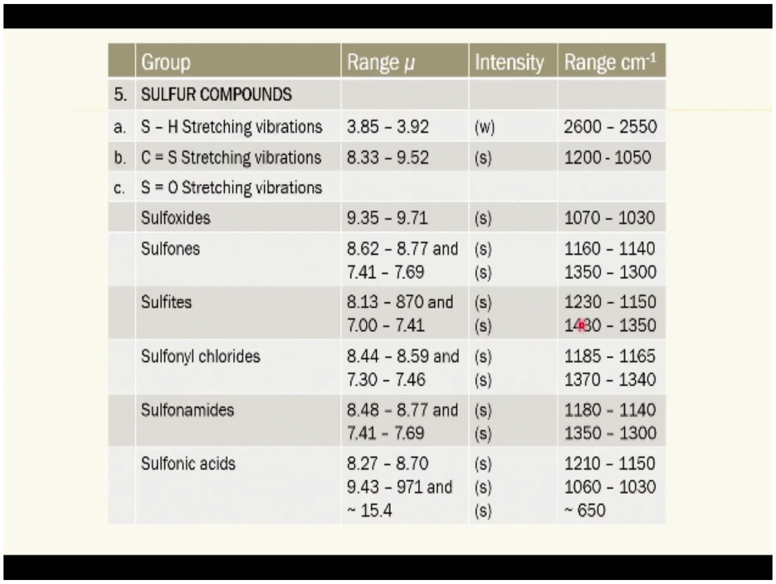

	Group	Range μ	Intensity	Range cm⁻¹
5.	**SULFUR COMPOUNDS**			
a.	S – H Stretching vibrations	3.85 – 3.92	(w)	2600 – 2550
b.	C = S Stretching vibrations	8.33 – 9.52	(s)	1200 - 1050
c.	S = O Stretching vibrations			
	Sulfoxides	9.35 – 9.71	(s)	1070 – 1030
	Sulfones	8.62 – 8.77 and 7.41 - 7.69	(s) (s)	1160 - 1140 1350 - 1300
	Sulfites	8.13 – 870 and 7.00 - 7.41	(s) (s)	1230 – 1150 1430 - 1350
	Sulfonyl chlorides	8.44 – 8.59 and 7.30 - 7.46	(s) (s)	1185 - 1165 1370 - 1340
	Sulfonamides	8.48 – 8.77 and 7.41 - 7.69	(s) (s)	1180 - 1140 1350 - 1300
	Sulfonic acids	8.27 – 8.70 9.43 – 971 and ~ 15.4	(s) (s) (s)	1210 - 1150 1060 - 1030 ~ 650

Now I will show you some of the IR peaks.

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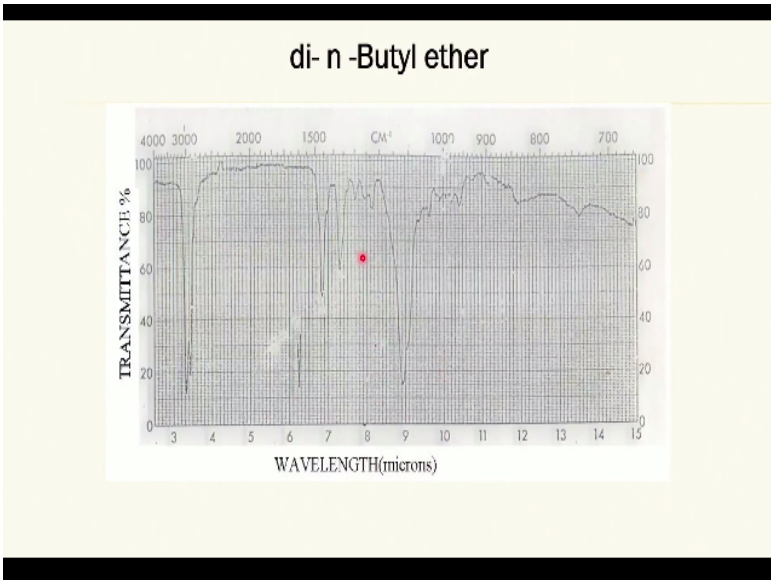

di- n -Butyl ether

There is this di-n-butyl ether you can see so many peaks here stretching frequencies and then because it is ether you will even see C-O stretching frequency and here most of them are wavelength that is centimeter, microns and centimeters inverse is put at the top and what is plotted is transmitted. This is for di-n-butyl ether ok.

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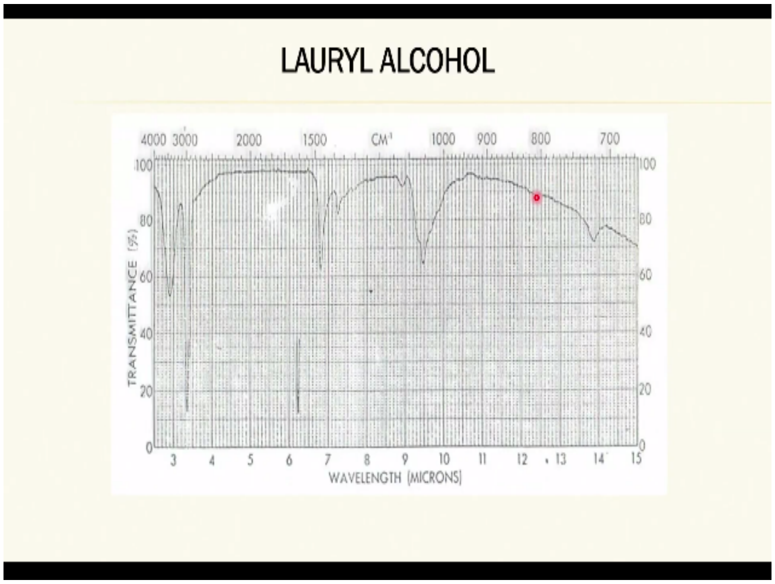
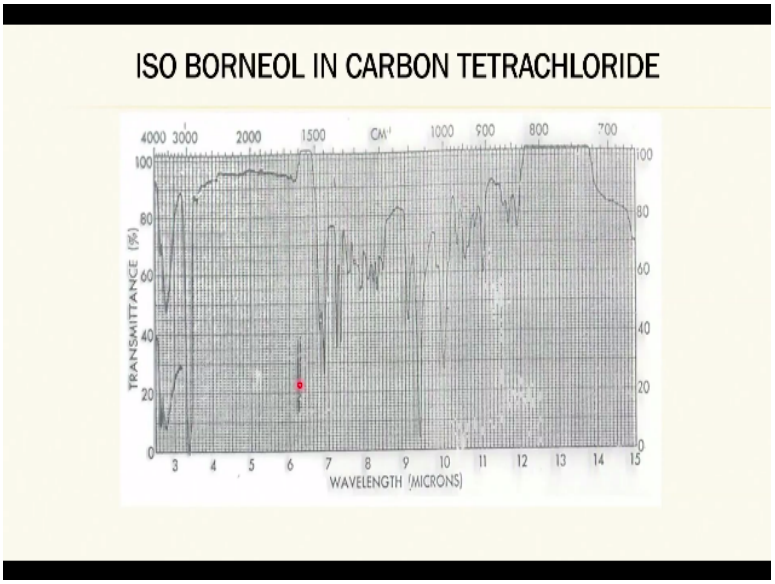


LAURYL ALCOHOL

Now you can see some more this is lauryl, you can see the peaks C-H stretching frequencies and then O-H stretching frequency is here, then there is one more O-H bending here, then there is CH stretching frequency is here like that because these are all given compounds spectrum has been taken, that is why we are able to identify. But if I do not write this lauryl alcohol one may be getting confused ok.

(Refer Slide Time: 26:46)



ISO BORNEOL IN CARBON TETRACHLORIDE

So Borneol this is the fragrance compound you can see the different peaks I suggest you try to write down the number and try to identify some of the peaks depending upon what I have taught you so far. So it will help you understand many peaks, IR peaks how to work with I infrared spectrum.

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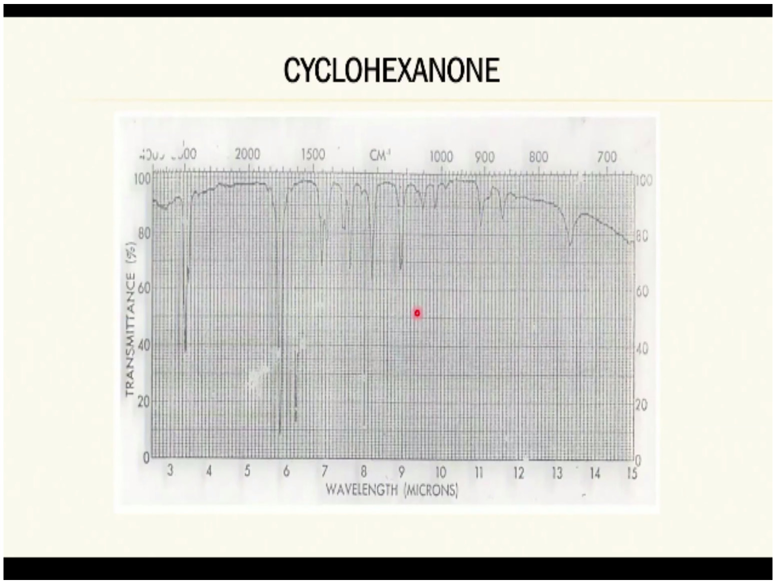

CYCLOHEXANONE

So this is cyclohexanone very well known compound and you can see one here and then so many small peaks here weak, these are all weak peaks, these are stretching frequency very sharp and if there is a broad peak like this it means there is lot of water in the sample ok in this range that is 2000, 3000 to 4000 range or we will show you some of them.

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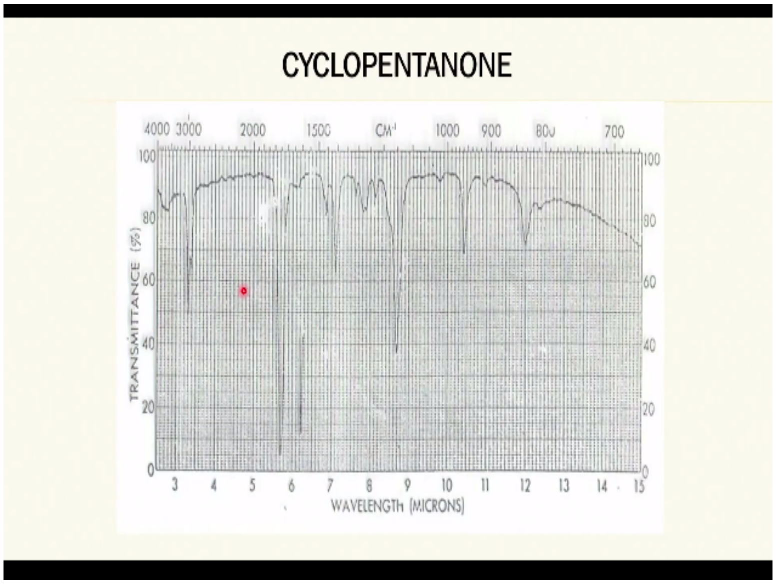

CYCLOPENTANONE

So this is cyclopentanone and very simple straight forward.

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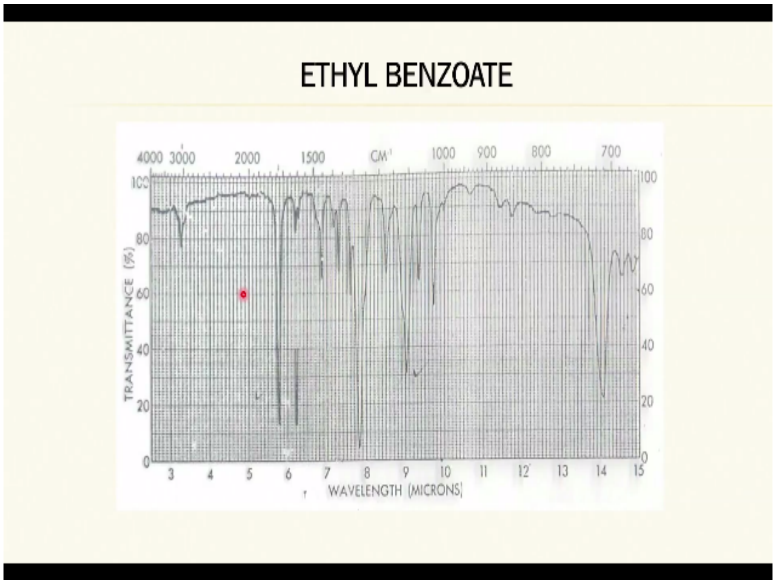

ETHYL BENZOATE

And then ethyl benzoate another infrared spectrum.

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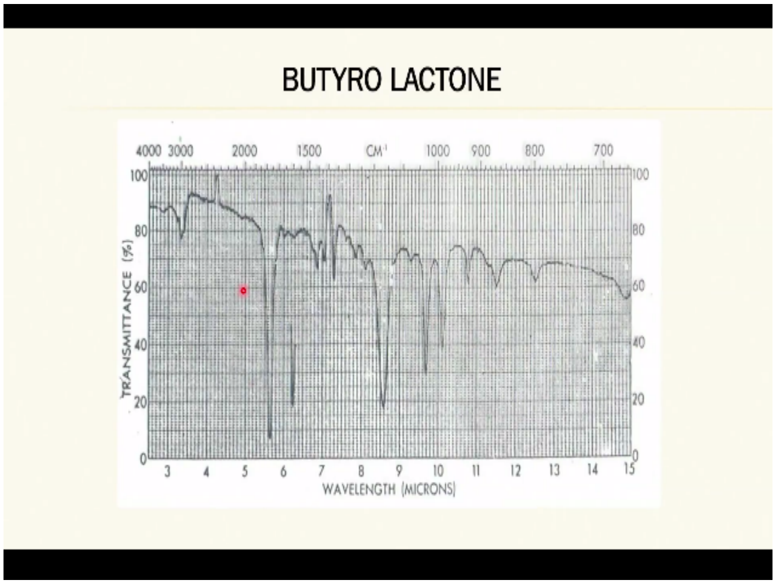

BUTYRO LACTONE

Then butyro lactone lot of peaks.

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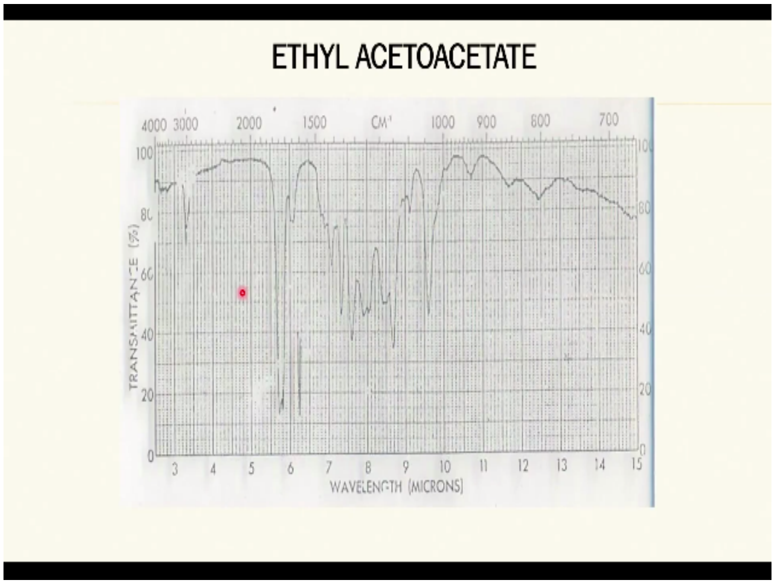

ETHYL ACETOACETATE

Ethyl acetoacetate these are only for your record, it will not be there for examination nor any related activity ok.

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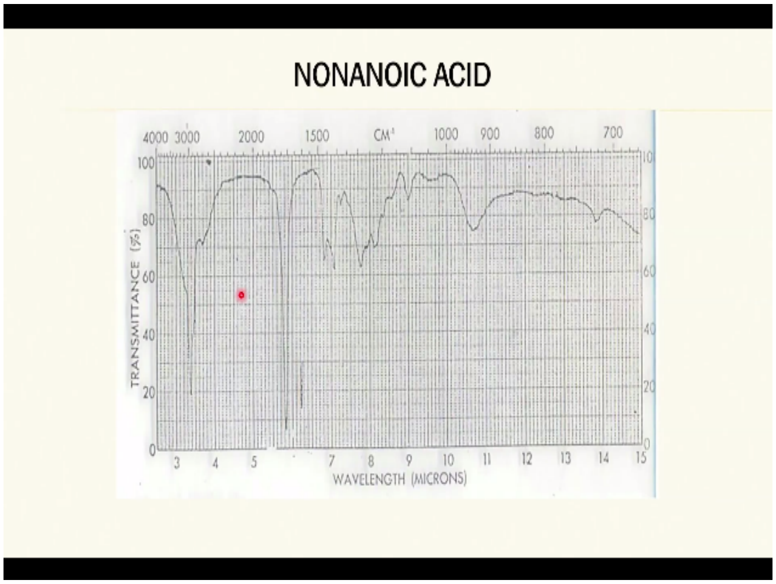

NONANOIC ACID

So nonanoic acid.

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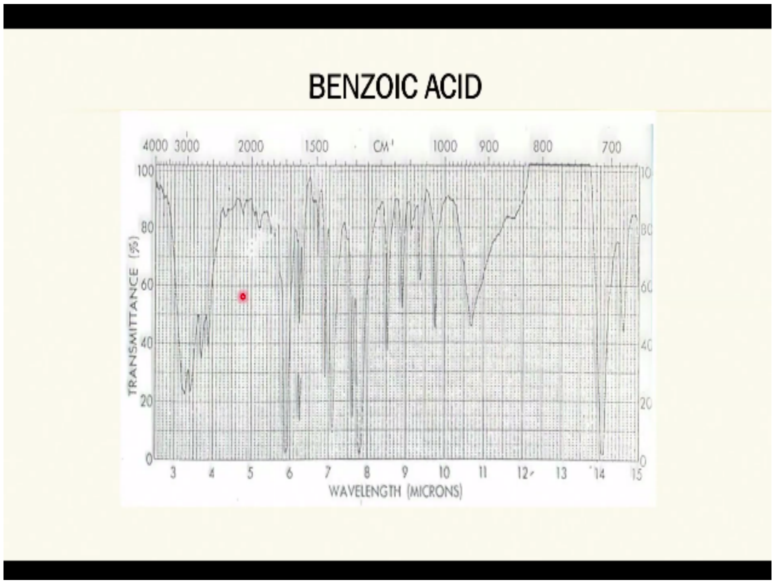

BENZOIC ACID

Benzoic acid is here, so some of these compounds when they are produced industrially we use these spectra for comparison for the purity ok. I now I would like to teach you about quantitative analysis of infrared.

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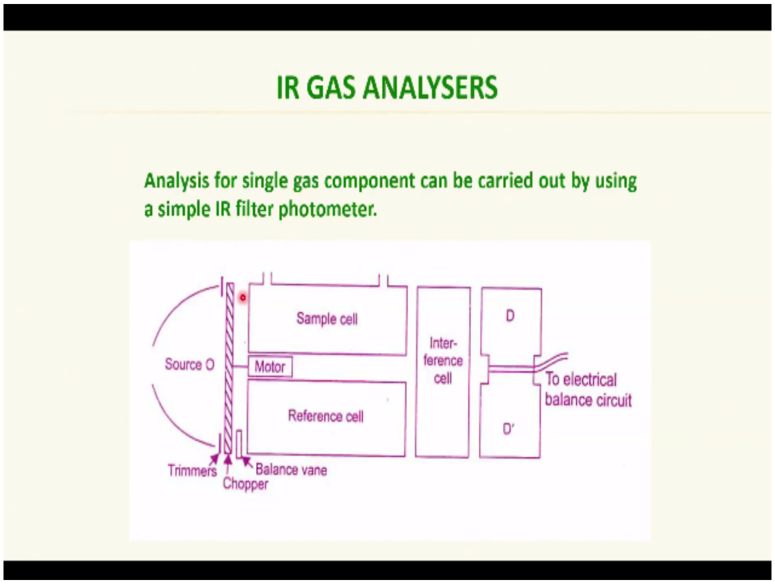

IR GAS ANALYSERS

Analysis for single gas component can be carried out by using a simple IR filter photometer.

That I will teach you in the next class ok, that all now we are almost nearing the end of our discussion and I will be concluding the session with IR gas analyzers as well as the quantitative analysis that we will do it in the next class, thank you very much.