Infrared Spectroscopy for Pollution Monitoring
Prof. J.R. Mudakavi
Department of Chemical Engineering
Indian Institute of Science-Bangalore

Lecture-01
Introduction to Analytical Science and Infrared Spectroscopy

Hello students, it is my pleasure to be here once again in front of you, earlier I have given 3 courses, 1 on spectrophotometer that is a 20, 30 hours program on NOC and NPTEL. I think then I have done one atomic absorption spectroscopy that is also about 30 hours and then 1 more course on ICPEAS inductive couple plasma atomic emission spectrometry that is for about 10 years.

Now I have decided that most of my MOC courses should be about 10 years not more than that because one thing is because they are all involved spectroscopy and atomic structure etc. and number 2 I would like you to participate in the total understanding of the subject that is the reason why quite often whenever I am doing a course you will see that lot of things are if you have taken my earlier courses you will see that lot of my slides are coming again in the new courses.

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There are 2 reasons for this, one is I can there are always new students appearing for the course and many of them are engineer, actually this course has been designed for engineers and other

professional who are not basically chemist, it does not mean that the course is not meant for chemist, it is meant for chemist also and especially useful for the students of M.Sc. chemistry, M.Sc. environment, M.Sc. Botany, Zoology etc.

And it is useful for the students of engineer, all engineering college students of metallurgical Engineering and then mechanical engineering and then chemical engineering and environmental engineering. So if I have such a wide background of students it is very natural that their background is also different but the subject is quite vast and specific. So what happens is quite often have to teach the fundamental.

Otherwise if I straightaway go into the subject there is always a possible that people many loose interest because they are not able to connect with the possibility with this subject. Quite often if you do not connect to the subject it leads to sort of loss of interest and secondly when you study the subject it is better to understand the subject in all its entirety, quite often name for example spectroscopy if you want to study.

You have to know about atomic structure, without atomic structure where is spectroscopy, but quite a few engineers and professionals who are well within their middle age and other practitioners who are into the monitoring business either in petrochemical industry or chemical industries or environmental agencies or any other environment related techniques. There is always a possibility that they might have forgotten or they might not have studied the subject all together.

Therefore what I felt is normally it is important for us to study the subject in all its entirety as I told you earlier. Now this topic which I have chosen infrared spectroscopy for pollution control monitoring etc. actually it is a spectroscopic technique. This spectroscopic technique obviously again it depends upon the atomic structure. Therefore it is very important for us to study the atomic structure and then maybe a little bit about the instrumentation.

And then about the basics of spectroscopy and then basics of infrared spectroscopy and then instrumentation of the infrared spectroscopy and then about the working of the spectroscopy, IR

spectroscopy followed by how to take the spectra, how to interpret, what are its applications and several other aspects of infrared spectroscopy. Now it does not mean that the whole world is composed only of infrared spectroscopy.

Otherwise there that itself could be a very special topic by itself. Now I have done earlier as I told you one on spectrophotometry, one on ICP-AES one on this atomic absorption spectrometry. Now spectrophotometry is a molecular spectrometry course it is also known as colorimetry, photometry, spectrophotometry and many other related things, they are used for different purpose. All spectroscopic techniques basically serve for the chemical analysis using instrumental methods.

We do not need the wet chemical analysis that means like a laboratory you do not have to take the sample dissolve it and then evaporated and there are many chemical processes involved in the chemical analysis, but spectroscopy as such has got an advantage that you do not have to do much pre preparation of the sample, straightaway we can collect the sample and do the analysis in 90% of the cases.

Remaining areas remaining cases there is certain amount of chemistry involved, it is inevitable see basically pollution itself is part of chemistry. Now a days lot of people do claim inheritance to pollution of expertise in pollution control, there are engineers, mechanical, civil, engineer, Electrical engineers for the maintenance of electrical equipment's and then chemical engineers want to have a big pie of that.

And then there will be automobile engineer, aircraft engineer, metallurgical engineers, so many other people who are working actively in pollution control. Now look at it from the scientific science point of view where are the scientist involved in the pollution monitoring scenario. First of all you would understand that there are chemist who are the who form the biggest chunk of the people who are interested in the environment.

And then there will be botanist, zoologist, and then physicist, there involved a little bit of mathematics people, there also involved geologists are involved and like that several other

scientists are all in involved, biochemist, pharmacist, quite a few people are interested in the application of such techniques in the pollution control area. Now if it was only scientists and engineers it would have been a fairly decent group to manage.

Now you will be surprised to know that there are lawyers, then are social scientist and there are economist and then there are other types of geography people, all kinds of people lay claim to the inheritance of pollution control and towards their responsibility. But again finally when it comes to the nitty-gritty of the sample analysis, handling and then day today usage etc., everybody will move away leaving the field open for chemist why.

Because most of the time spectral techniques as well as environmental evaluation, that is the trace or ultra-trace or it is in macro or micro several other types of analysis which form the bulk of the environmental pollution control activities. They are all dependent upon the concentrations of the substances in the environment. Once these concentrations are known then other things can be planned, but first of all to know the concentration of a pollutant we have to know we have to feel the effect personally.

Then only you will say that ok yeah this compound is harmful, this compound is not harmful etc. and then again there are gradations. For example there are pollutants like cyanide any quantity smallest quantity you known even in PPM level it is lethal, you all of you must be remembering the Bhopal incident where methyl isocyanate as a gas protruded at night in 1984 15000 people died, the concentration that is lethal concentration.

Nowadays only we know at that time nobody knew what is the lethal concentration, how much you need to take before the melodies effects, melody of visible. Therefore the analysis of the pollutants always forms some sort of basis for the assessment of pollution and luckily chemists are trained to do this. Chemist work on normally 3 or 4 levels of determination and chemist are like gods you they can do anything.

A good chemist will do not only chemistry, but he can contribute in mathematics, in physics in several botany, zoology etc. etc. in engineering, in mathematics, in modelling etc. But the reverse

is not true. For example a good mechanical engineers even though he may be contributed in the field of pollution control, if you ask him something about the chemical aspect he will draw a blank, he will not no, no, I do not know that is not my area something like.

So you should always be a little biased towards chemistry especially when you are dealing with the environmental pollution control, that is my specialization, my name is Dr. J. R. Mudakavi I am from the department of chemical engineering Indian Institute of Science Bangalore and those of you who have attended my course will know that we have done lot of work on the concentration in chemicals etc.

We will repeat part of it in this but not all. Because in this course I am going to concentrate mostly on the infrared spectroscopy, but again since we are going to work on quantitative aspects we have to work on 4 levels as I was telling you, 1 is major components and second is minor components ok, third is trace component and nowadays there is a fourth component that is ultra trace components.

So you widely classified we can say that major components are those components of an environment matrix, it may be near matrix, it may be a water body, it may be soil body or anything ok hazardous waste body. So the such matrix matrices we have major component up to 1% ok, so 1% and above we call that major component because most of the such analysis can be done by wet chemical analysis in a laboratory you can carry the sample do the analysis give the result.

And apply it wherever is applicable, then comes the minor component. Now the problem with minor trace and ultra trace components is the matrix components that are not required for analysis form the bulk of the matrix. So it is a as you go down the concentration range for example from 1% let us say 0.1 to 0.2% pollutant is there in 0.1 to 0.2%. The remaining part is a bulk of the matrix that has to be either removed or it has to be made in effective in the technique what we are using.

Now the problem becomes more difficult when we reach the trace levels and what are trace level, trace levels are in microgram, microgram per gram or milligram per kg or so many grams for ton per ton like that they are all in same SI units, there is nothing hard and fast rule but most of them are in parts per million maybe sometimes sub parts per million.

That is part per million means in about 10 raise to -6 grams that is the weight range 10 raise to -6 grams per gram that is microgram. Now sub microgram would be less than that, we do not go to 10 raise to -9 level because that comes in the ultra-trace levels. In ultra-trace level we want to determine concentrations of pollutants in about 10 raise to -9 grams that is the absolute level. So from the absolute level 10 raise to -9 level.

The range extends up to 10 raise to -12 that is from nanograms to pico grams ok and then sometimes you will come across areas where still lower concentration are required for chemical analysis, that is the biggest challenge. Now what happens as I go down the concentration range the matrix component looks huge, is not it 10 raise to -9 remaining all in grams, so it is like finding needles in the haystack.

But there is one difference these needles whatever you want to do is we want to catch them and count them see it is not just finding qualitatively the needles are there or not. But we want to know how many needles are there, that is finding how many needle sticks are there in a big huge bunch that is the challenge. So the more and more we want to work at lower concentration levels the challenges become much more insurmountable.

But as I told you chemist are fairly intelligent people they are like gods, they think differently, the act differently, they know how to solve a problem given a problem, they know how to solve the problem. So in my course what you will be learning is this about the infrared spectroscopy application. Other techniques you can always go through my earlier NPTEL courses I am sure they will be available at IIT Madras and the IIT, IISC and other database centre.

But this one is new one and you can go through them both all spectrophotometry ICP and atomic absorption. You know this is the fourth one, I will try to make this a fairly simple and straight

forward because there are engineers non engineer, chemist and non-chemist all are involved. So sometimes for the people who are well trained in chemistry it maybe a little boring because (FL) what is this he is teaching same material, electrons, protons etc.

But I feel that it is time well worth spent because you are not going to spend too much we just going to refresh our memory regarding the atomic structure study and then we will study about the fundamental. I also have to bring out the significance of the environment with respect to infrared spectroscopy ok. This is environmental pollution, so apart from instrumentation we are also going to concentrate on how to determine the organic compounds in a given matrix.

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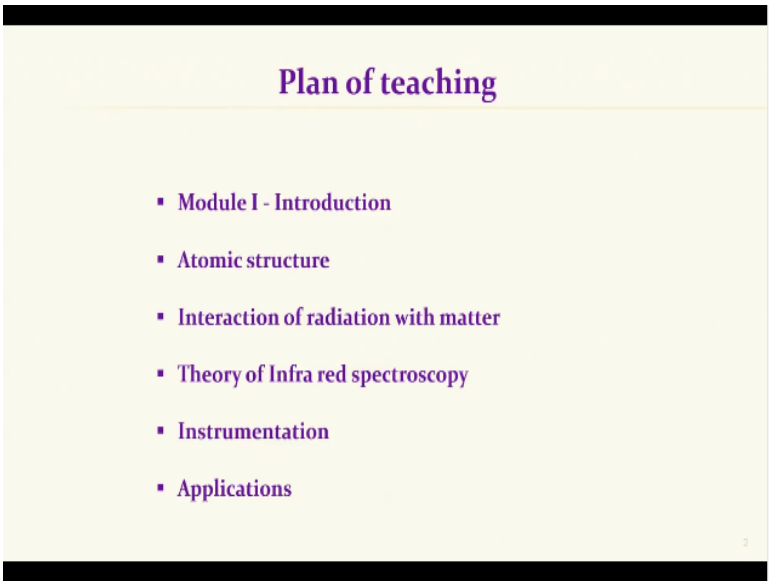

So this is the plan of the teaching, what I will be teaching you, first is module 1 that is introduction and then second next module is about atomic structure and third is interaction of radiation with matter because all spectroscopic material techniques usually involved interaction with matter, matter means it may be as mirror, it may be a glass, it may be an instrument, it may be an electron many other things are in involved.

And then with this general introduction we are going to spend some time on the theory of infrared spectroscopy, how does infrared spectroscopy originate ok. So that we will give you a firm basis on the infrared spectroscopy then you will study the instrumentation, and finally the

application of infrared spectroscopy. Now in this series of programs I want you to understand this is the sort of credit based course ok.

So there is no compulsion for you to take the examination or assignment, but they all form part of the MOOC program as finalized by the government of India IIT, IISC then all these people are involved in the program finalization. So I strongly urge you and go through the process of assignment and final examination. In this course I am going to make it only something like online examination, not offline.

That means you will be writing just online examination, just like you are coming for a class and finished exam and go. Whether you do well or not depends upon how seriously you are studying this subject and usually we have about 40% questions from the part 1 no maybe more than 40, up to 50% questions are from the taught courses and it will be like this just you and I talking and you learn the subject, same questions will come or you can save the material by as and when I am giving the lecture, you can record it and study it then come back.

And then there will be certain amount of test for intelligence and if you are I do not expect you all to be 100% chemist and I do not expect you all to be 100% you know genius chemist or engineers chemist for that matter, but there will be opportunity for you to exercise your brain, you know it is not meant for hi-tech engineers or hi-tech chemist with ordinary background with what I am teaching you will do well in the course.

And I expect you all to take part actively in the course. So that we all learn it well. so once you know this is subject, you know you are ever ready for the challenge that comes if you are a student in your class room, in your examination or in your future career, if you are in industry, if you are using it will always come in handy. So let us get on with this and then what I would like to do is to spend some time regarding the introduction.

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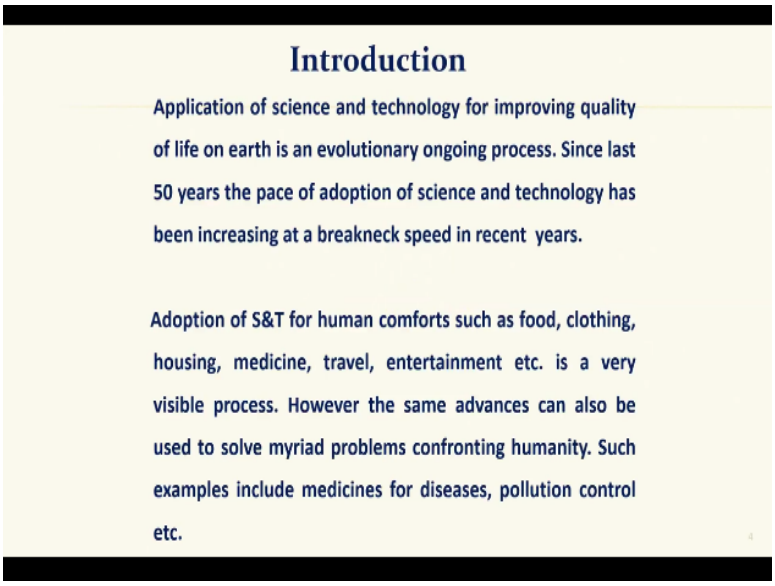

Because introduction again apart from what I have told you already there are certain other things involved in the introduction, that is why I want to spend some time ok. So this is the introduction what I wanted to tell you, this is a very general introduction ok. So general introduction means we are going to talk about environment science technology world this, that pollution etc. etc. SO we have my first sentence you can see that it is there application of Science and Technology for improving quality of life on earth is an evolutionary ongoing process.

I think you all appreciate this sentence, so science and technology is required, it is meant for improving quality of life of ours, yours and some other animals maybe underwater, over water, in the forest elsewhere whole life as such, that is a revolutionary ongoing process, because whatever development, whatever we call as development means changes from the existing systems.

So any change in the existing system always comes with the plus and minus part of it ok. So sometimes according to Darwin changes his are meant for the fittest and according to Mental Lamarck, according to Lamarck changes for the better will be carried on to next generation or future generation, if the changes are beneficial to the species very very interesting topic about the evolution of life, please read out Lamarck's contribution today evolution of life.

In addition to Darwin, Darwin that we all know how he makes it etc., but as and when we introduce changes in our life, there are going to be used and profound changes will happen. For example if I introduce car in 1800 1780 was the first car that was produced in America and now we have so many millions of cars on the road definitely it has worsened the life of the environment work has worsened the life of the insects and many other things.

And our the quality of our year also has worsened, but it has also given us something you know to enjoy, you can travel faster, we can travel safer, we can travel without much problem like that there are always changes associated with evolution and development that is there one of my main theme and analytical science is no exception, we have developed wonderful techniques over the number of over number of years especially since 1960s.

I am a product of 1960s to 80s and then I had taught in the Indian stuff science for 36 years and I have seen the changes coming and you know differences people changing for particular species, particular analysis how people go about doing it takes it ok. So since last 50 years as I told I was telling you the pace of adoption of Science and Technology has been increasing at breakneck speed, I think all of you remember your mobile right.

So in 1990s mobiles are introduced you know just very primitive models, now a days I call a simple mobile as Gandhi Engineering Mahatma Gandhi be used say that we should do more it less, now the mobiles have becomes smaller, they have become thinner, they have become more complex, but you can do many things with the mobile is it not, there are mobiles which can do internet for you, mobile which can capture your image, self they can capture your selfi image ok.

They can send messages, talk to somebody on the phone, collect data, do literature survey and then many other things in are there must be about 6 to 8 million applications of software apps, I think all of us are familiar, but just imagine a case of a water mobile about 10 or 15 years before mobiles they look like primitive mobiles is not it, so this breakneck speed of change in the environment in our life occurs or it occurring very fast, even for our comfort.

So the adoption of Science and Technology for human comfort are also increasing there is requirement of food, there is requirement of clothing, requirement of housing, low cost house, high cost housing, all kinds of housing, medicine, travel, entertainment, and many of these. So it is the very visible process basically right. So however the same advances can we use to solve myriad problems, confirm to humanity, we can cite several examples green revolution.

White revolution and then include medicines for diseases, pollution control, several other disciplines have emerged over a period of time to solve the problems of the society which may be of recent origin or may not be recent origin. For example many of the efforts are under the impression that the pollution problems are all man made no not at all ok. Now if you think it is only the man-made problems that we are facing it will be an absolutely wrong conception.

For example there is lot of Sun's heat and other things are there which had made changes in the environment of the earth several thousands of Dinosaurs and other life forms exformed and extinguished so many cold climates have coming, so many changes have taken place. So it that has no meaning to say that everything is of anthropology origin that is not right. So look at it like this, fundamental sciences such as atomic and molecular structure.

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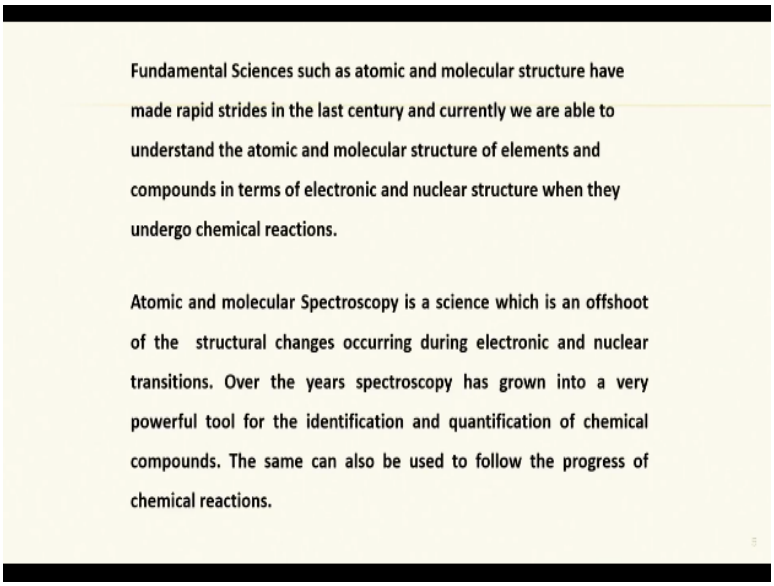

They have made rapid slight strides in the last century ok, this I have been emphasizing because most of the understanding of our nature comes from the understanding of the chemistry ok. So

this currently most of our knowledge comes from development since last 200 years, people have been trying to record or determine understand the structure of the atom, structure of molecules.

All those things since 1800 right yeah sort of and in currently we are able to understanding atomic structure, molecular structure of elements and compounds in terms of every electron that is involved in the building of the molecules and elements even though we do not see the electrons, we can still predict what it is made of, how the electrons are arranged etc. and we can produce nucleus structure.

We can play with the nucleus structure, do fission, do fusion, do many other things make them undergo chemical reactions, produce energy, and many other things, so atomic and molecular spectroscopy again is part of the development of our understanding of the atomic structure. So it is a science which is an offshoot of the structural changes occurring during electronic and nuclear transitions. So all the basis of spectroscopy is the changes in the electronic and nuclear structure.

Sometimes we are solely dependent on upon the electronic structure, electronic transitions, electrons escaping, ionization and all those things are there and sometimes we expect the nuclear changes to occur alpha, beta, gamma, radiation changes etc. They are also they are occurring during the electronic and nuclear transitions, so over the years spectroscopy itself has undergone changes quite a lot during electronic and nuclear transitions.

Our spectroscopic technology or knowledge has grown into a very powerful tool for the identification and quantification of chemical compounds. The same can also be used to follow the progress of chemical reactions also. This is one advantage of how we are going to improve the quality of life whenever I want to carry out a chemical reaction you want to know how far a reaction proceeds.

So how do you do that, most of the time you have been trying to take the sample analyze it etc. but spectroscopy has made the job very simple to just take a small sample put it in a spectrophotometer or spectroscopy tool, it will give you the progress of the reaction ok. So we will continue our discussion in the next session.

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What I wanted to tell you in this case is that the spectroscopy is part of our life today, it is useful for myriad programs ok, my next slide I am going to talk about environmental pollution.