Circular Dichroism and Mossbauer and Spectroscopy for Chemists
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Lecture – 35
CD Spectroscopy: Conclusion

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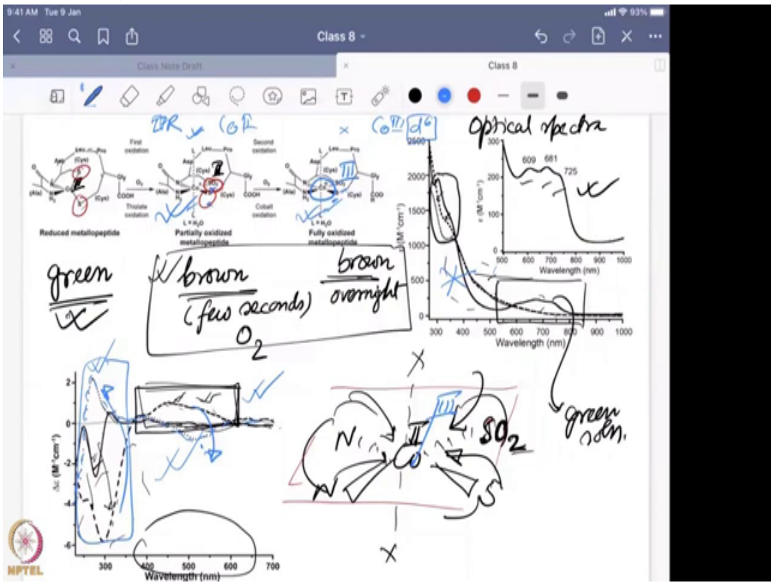

So, with that we come to the end of the CD spectroscopy discussion.

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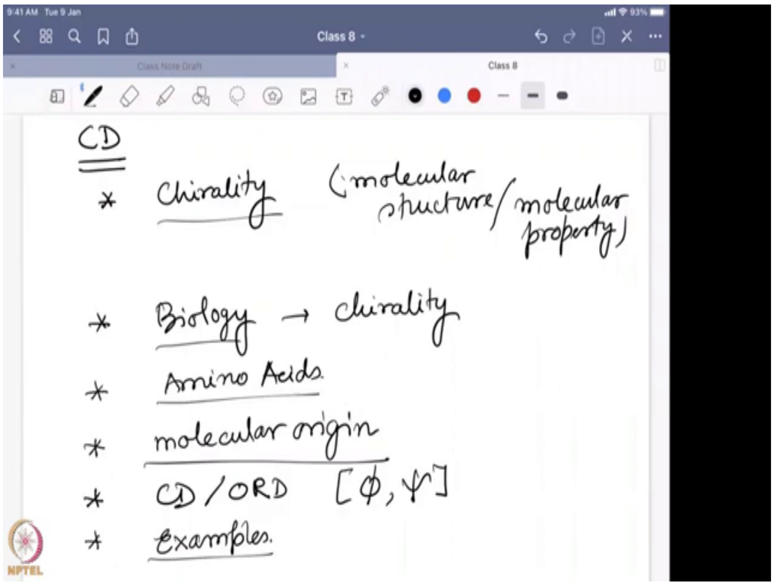

CD

* Chirality (molecular structure/ molecular property)

* Biology → chirality

* Amino Acids

* molecular origin

* CD/ORD [ϕ, ψ]

* examples.

So, in the CD spectroscopy discussion we have gone through these following points. First of all, why chirality is crucial? Because it connects molecular structure with molecular property. Then we look into the system why it is important? Because biology actually plays with chirality. So, chirality is an important factor over there for controlling the molecular recognition controlling the reaction rate.

Even you can say chirality is a signature of biology. If you have an enantiomeric excess of a sample, you can say it is probably something biological is influencing over there. Then we look into especially the amino acids. So, study the amino acid structure, there one letter and three letter codes. And how it is happening? So, we actually, gone through them and then we looked into the molecular origin. Why a system can be chiral?

It is coming chirality from not only the molecule but also the light. What is the LCP and RCP? How it is behaving? Then we found some of the parameters that we can use CD and ORD which is coming from optical rotation and the ellipticity that it is coming. We found CD is actually a better parameter to find out the chirality of a molecule. And at the end, we have gone through some of the examples of chirality.

And how it can help us to not only know the overall the structure of the molecule but their stability, whether it is binding a metal or not and all this particular information. So, these are the take home messages from the CD spectroscopy. So, please go ahead and ask any question if you have any before we go for the next topics. So, please go ahead and ask any question if you have any or any comment.

That you want to repeat some of the topics one more time or you are not very happy of the explanation of the few topics you want to go ahead with one more time, please go ahead. **"Professor – student Conversion Starts"** Sir previously, yesterday means that in the previous class we have told that about the directionality. So, what is the means X polarized light, Y polarized light and Z polarized light? And how we will distinguish them?

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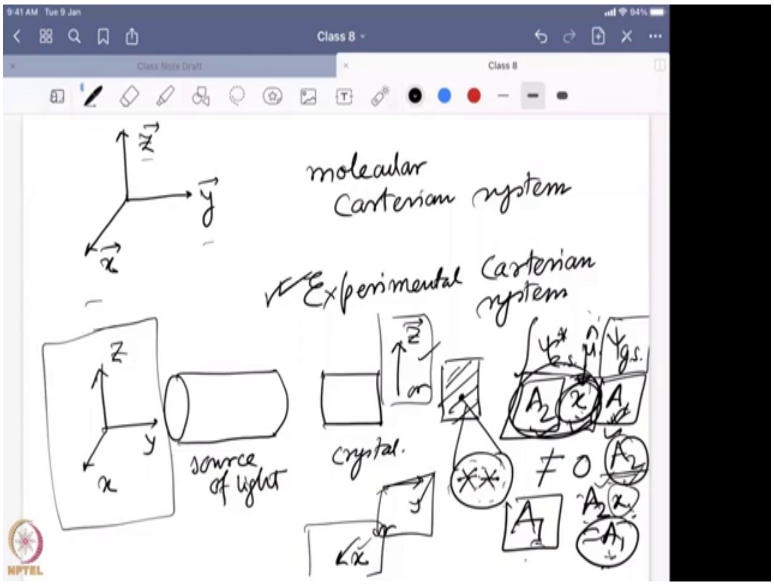

So that is a very important question that is mostly going to be covered in professor Leela's class. So, I am just going with just a hint of it. What is X and Y is equivalence like? So, when we actually, do look into a system we try to look into a system in a Cartesian axis. So, we say so, this will be my Z axis, this will be my Y axis, this will be my X axis. However, the molecule is always stumbling.

So, there are two different accesses you can think about one is actually a molecular Cartesian system and the other one will be your experimental Cartesian system. And this all difference between them is how you define your X Y Z axis? Which direction? What is the angle? And all those things now, in the molecular Cartesian axis is a bit difficult to define because the molecule is not remaining at the same place altogether.

Unless, you go to 0K and even then some vibration will be there. The molecule is not going to be stable. It is undergoing different motion, vibration, rotation, translation. All together, you can see it is going to **(()) (04:24)** motions. So, you cannot define a molecular axis all the time very clearly. So that is why what we do in experimental system? We actually, specifically define this is my X Y and Z axis.

And depending on that I actually, measure all the different samples in that experiment. And whenever we define an X Y Z axis, it means I am defining it with respect to experimental Cartesian system. Now, over here in an experimental Cartesian systems let us say this is your source of light. And this is actually a crystal that you put to create your linearly polarized light and here is your sample.

Now, in the sample if you look forward, there are different molecules and they can have different orientations not all of them are going to be same. And how I am going to define it? So, I am going to define it with respect to the X Y Z axis of my experimental system. And over there, I am saying that I am going to put my crystal such that I am going to get only this axis or this axis or this axis.

So, with respect to that I am going to say, I have X polarized light, Y polarized light and Z polarized light. And over there, the molecular motion is quite fast and the interaction and time I am giving to this molecule for this optical spectrum. It is happening in the millisecond to even second scale that is my time region. And within that time a molecule will be very similar to the X Y Z axis of my experimental section for a while.

And in that time, if it is there, it will absorb the light, depending on whether it is Z Y or X polarized light active system. Now, how I can define that which particular transition is X Y Z alive? For that system, again you have to look into the transition moment integral look into your excited state operator and ground state. And what you need to look into? What is the symmetry representation?

Ground state you can say like it is a Π-Π* these two σ* all this interaction, each orbital you can find out with respect to the symmetry element present in that particular point group. What is that symmetry representation? Say it is A_1 say it is A_2. Now, A_2 and A_1 all together if you want to have it to be non-zero, whatever is the symmetry representation of μ. All these things should come together and give a non-zero system.

And it is only possible in one particular condition. It has to be the A_1 the totally symmetric representation for that particular point only then it can be non-zero. That means you have to find out the X such a way that it will be multiplied with A_2 and A_1 and give you A_1. And that is very easy because from the point group again you will learn all those things in the later part of the class.

It says if you want to have a A_1 it is only possible if you multiply the same system to A_1 that means A_2 and X should be A_1 together and only then A_1 into A_1 give you A_1. If you multiply anything else B_1, B_2, A_2 with anything with the total symmetric representation A_1 we are going to get back that particular representation. So that means A_2 and X multiplication should give you A_1.

And the other corollary of the point group character table is if you want to have A_1 by multiplied by two different groups. It is only possible if you multiply the same system $A_{2\times}$ A_2 give you A_1, $B_1 \times B_1$ give you A_1, $B_2 \times B_2$ give you A_1. So that means the X has to be A_2 symmetry. And then you look into the character table find out along with the A_2. What is there?

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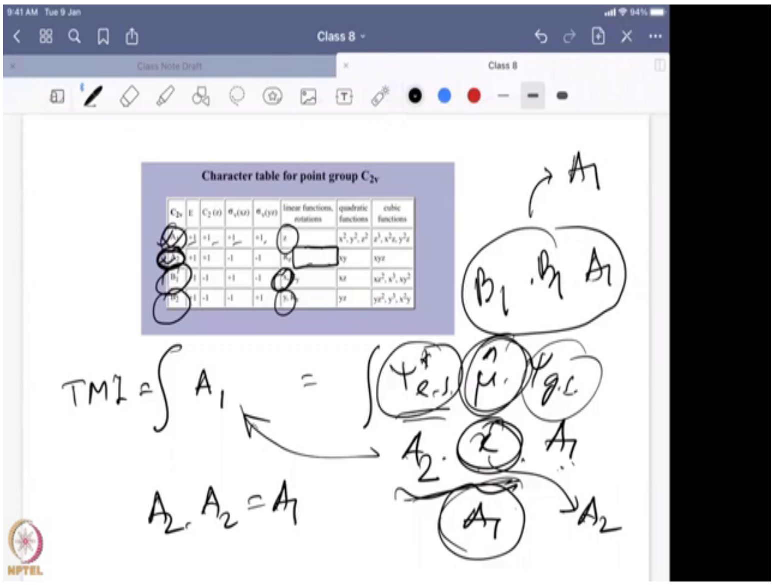

Character table for point group C_{2v}

C_{2v}	E	C_2 (z)	σ_v(xz)	σ_v(yz)	linear functions, rotations	quadratic functions	cubic functions
A_1	+1	+1	+1	+1	z	x^2, y^2, z^2	z^3, x^2z, y^2z
A_2	+1	+1	-1	-1	R_z	xy	xyz
B_1	+1	-1	+1	-1	x, R_y	xz	xz^2, x^3, xy^2
B_2	+1	-1	-1	+1	y, R_x	yz	yz^2, y^3, x^2y

So, for an example let me take a graph of that. So, say this point group of C_{2v} point I am talking about. So, over there say I find out A_1 is a totally symmetric representation and this is what I want after that TMI? It should be A_1 and say it is nothing but a ψ* state my operator and ground state say my ground state is A_1 my excited state is A_2. Now, I have to find μ such that whatever it is, multiply that and give me A_1.

Now, these two should give me A_1 together because you can see it is all 1, 1, 1. So, you have to multiply that thing with A_1 only then you will get 1, 1, 1, back totally symmetric representation. So, A_2 and X should give you A_1 that means it should be an A_2 symmetry because only $A_2 \times A_2$ can give you A_1. So that means it should be A_2 symmetric and look into there over here, you see there is no X Y Z.

So, no matter what polarization you give? This will be a transition that you will be never missing. Now, say my excited state is actually B_1 and ground state is still A_1 so then it should be a B_1 again. So that we can multiply all these things together and get an A_1 so, if it is a B_1 then it should be X polarized only then it should be happening. Similarly, for B_2 active system it should be Y polarized A_1 active system it should be Z polarized.

And by that you can differentiate which particular polarization is happening and if your molecular structure that you are imagining to behold a particular point group, it is true or not. Does it answer your question? Yes, sir. Thank you sir. Any more question before we close it up. **“Professor – student Conversion Ends”.**