Symmetry and Group Theory
Prof. Anindya Datta
Department of Chemistry
Indian Institute of Technology – Bombay

Lecture – 36
Symmetry of Normal Modes: A Shortcut

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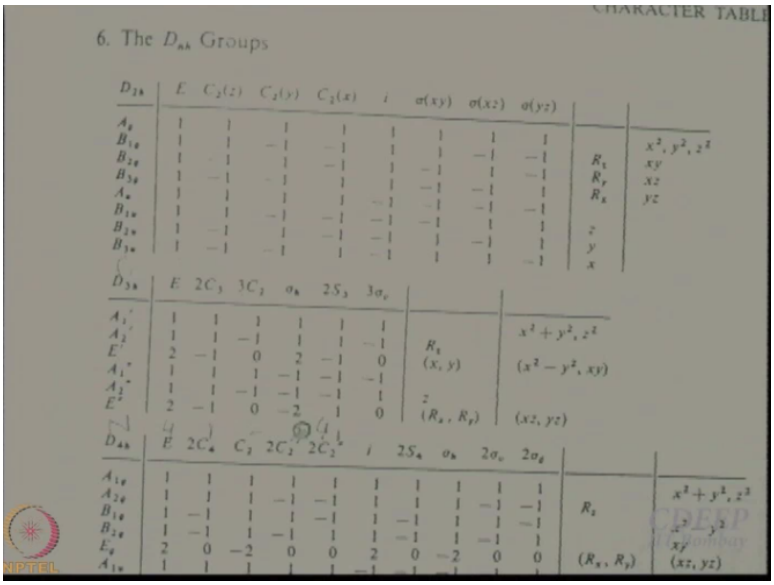

Can I simply things a little more? If I multiply by n instead of multiplying by n if I multiply by n - 1, what will happen? What will I get? What representation will I get if I multiply instead of n by n - 1. I will get gamma v + gamma dot. What I am saying is if we just multiply this characters of gamma xyz, by n, the number of atoms that remain unchanged, unmoved by the symmetry operation, then you generate gamma 3n that is far is everybody okay sure?

So say that why are leaving this difficult task of reading your mind to me. You understood n. You understand Dn, you understand gamma xyz. You know how I got gamma xyz sure. So now, if I multiply gamma xyz by n then what happens? n is the number of atoms that do not remain unchanged. For each of such atoms the character is going to be corresponding to a character of gamma xyz for any symmetry operation.

In gamma 3, how do you get gamma 3n. We got some identical blocks and so we just multiply it the number of atoms that do not change by the character of those blocks. Now already generated

the characters of those blocks by taking gamma xyz, so after all we are working with x, y, and z not fixed somewhere else but fixed to each end of the atom. So whatever transformation you make to x1 the same thing will happen to x4 if x1 and x4 happen to be the unmoved atoms.

So do you agree with me that gamma 3n can be generated by multiplying the characters of gamma xyz, by the number of atoms that do not change place. Alright. So far so good. So are you all ok with this. Even if you are okay with this it is easy. Then you how to generate gamma 3n then just subtract gamma dot and gamma xyz, from there you got it, but what I am saying is see this gamma cn is related to gamma xyz is not it. So chi (R) of gamma 3n = chi (R) of gamma x, y, z * n. Can I now move this out?

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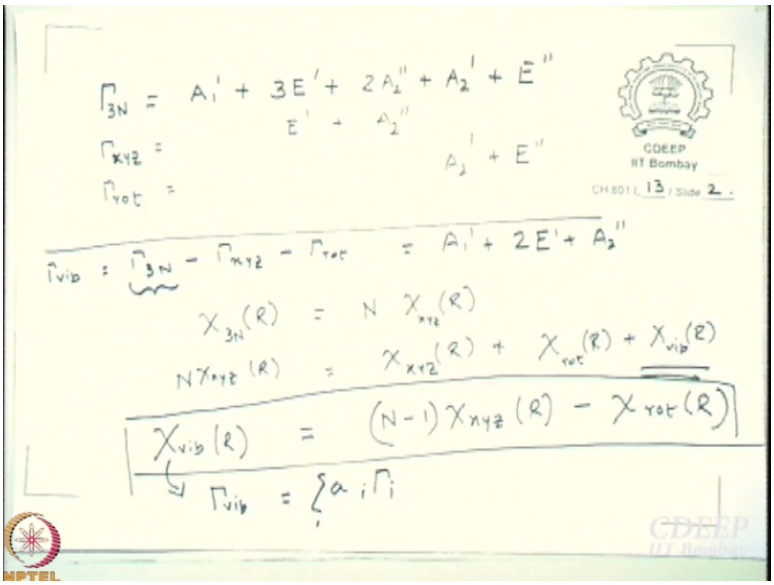

What I am saying is, chi (R) of gamma 3N = N * chi (R) of gamma x, y, z. So if I want so this, what is this equal to? This is = chi (R) of gamma xyz, + chi (R) of gamma dot + chi (R) of gamma with sure. So now is it easy to simplify a little bit or not. So I will write this here N chi xyz, (R) is this. What do I want? I want to know what is this? So can I not write chi vib of R = the exactly (N - 1) chi xyz (R) then - chi rot (R). Simplify the formula. Is not it?

So see what are we doing now? We started with things like unitary matrix, unitary representation, class, this that. Slowly we are moving towards the situation where we are generating a machine which can almost now work like a black box and give us answers even if you have forgotten

everything that we have learnt before mid semester. And that is the idea that is exactly what we want to do but we now try to generate some general formulae which people can use easily to get whatever answer that want.

So we like this formula or not. So if you work what is gamma vib? Work out what is gamma vib then. We have already worked out. So just check whether you get the same answer by this or not, so you should get the same thing. So basically what we are saying is that first work out this chi vib, generate gamma vib from there and then using your Ai = 1/h sum over chi (R) up data. Chi (R) formula decompose it into constituent irreducible representations.

Understood what I am saying. So all these chi (R) is going to give you gamma vib. Then you decompose it into sum over i * ai * gamma i. So that was 1 part of the story. Now what we want to do? See so far we have been able to perform symmetric classification of normal modes, but I do not know whether these modes are stretching mode so whether these are bending modes or what that is no fun. Just in case we you want to know which normal mode is which? Just if you tell me that this is the symmetry that I will not be happy with that.

So let us see whether it is possible for us to work out at least in a qualitative manner which normal mode has contribution or what kind of molecular motion. What are the different kinds of vibrational motions that you can think for bf3 or cu carbonate? What is stretch? What is the meaning of stretch? Bond lengths will increase and bond lengths will decrease. So you can also think of bend. Bend is also let us first say, in plane bend. Do you think of in plane bend? Bond angles will change; bond length will be remained the same.

And the third kind of motion would be the domain motion that we are demonstrating. that is out of length that is the only out of plane motion that can take place and now onwards are going to be the linear sums of these different kinds of changes in the different kinds of parameters changes in bond length, changes in bond angle, and out of frame motion. Which day is today? There is a class after this. Alright I will stop.