Chemical Kinetics and Transition State Theory
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Lecture 19
What is a transition state?

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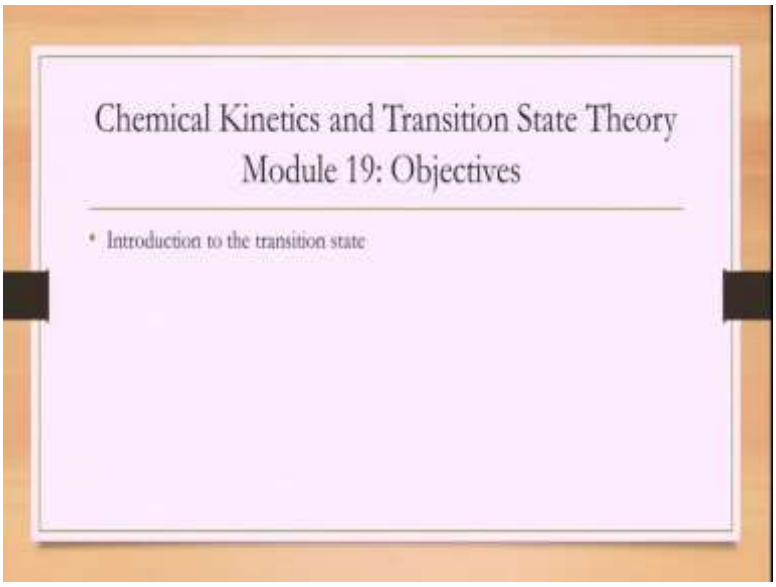

Hello, and welcome to module 19 of Chemical Kinetics in Transition State Theory. In the last several modules, we have been dealing with the partition functions for the sake of transition state theory. Today, I want to just take a little pause and want to describe one idea qualitatively which is the most important idea, by the way, which is what Arrhenius is famous for the idea of transition state. So, one of the critical assumptions made in transition state theory is that there exists a transition state.

So, today's module I just want to look into what is a transition state?

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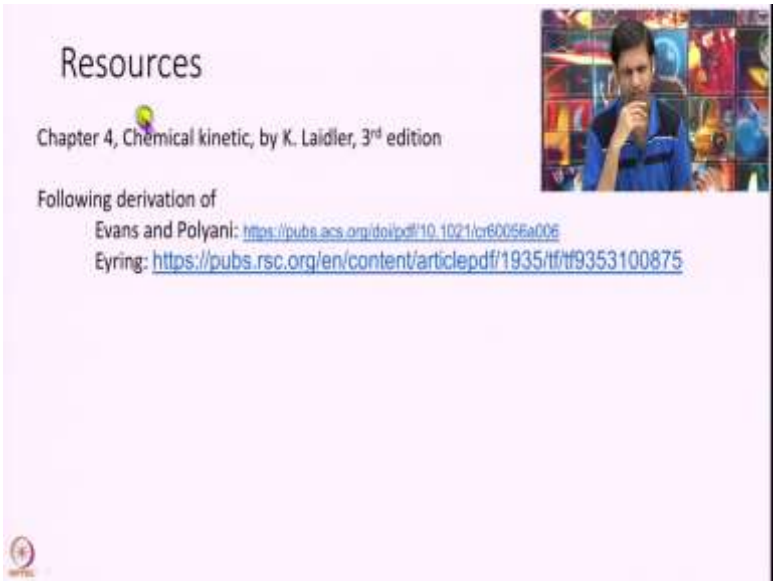

So, what we are following is the book by Laidler, the chapter 4 of the third edition, once more a different edition, you will find this in a different chapter number.

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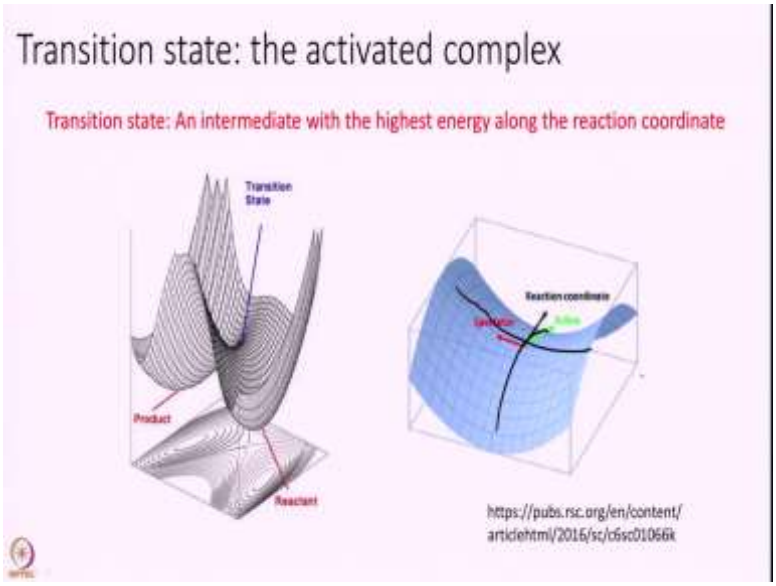

So, transition state is an activated complex in the language of Arrhenius, so transition state is an intermediate with the highest energy along the reaction coordinate.

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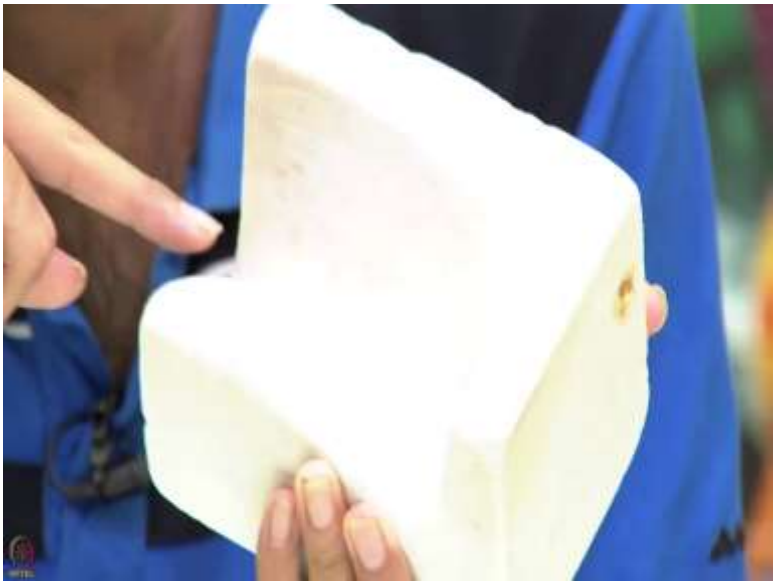

So, I have a little model with me, what this model is showing is a cartoon potential energy surface. So, what do you the idea is think of a reaction happening let us say this side is reactants it is a minima. So, this side is actually the products. And for the reaction to happen, you have to pass through this valley here, now to pass through this valley, your energy first goes up, and then it comes down.

So, this is how a complex energy surfaces look like. In your high school, you might have seen 1D surfaces. But this is now we have to think about more complex structures, which is in higher dimensions. This also is in only 2D, but you can imagine a much higher dimensional structure we have a reactant energy increasing and energy decreasing.

One important point here, which is a very big misconception among a lot of students, this point, which is the maximum energy along this line, is called a transition state. That is not the misconception; the misconception is that this transition state is not the maximum energy structure really.

So, if I look at this transition state, and imagine the dynamics along this perpendicular surface like this, that one transition state is the minimum energy structure. So, the transition state is the maximum energy structure only along the reaction coordinate and the reaction coordinate takes you from here to here along this valley.

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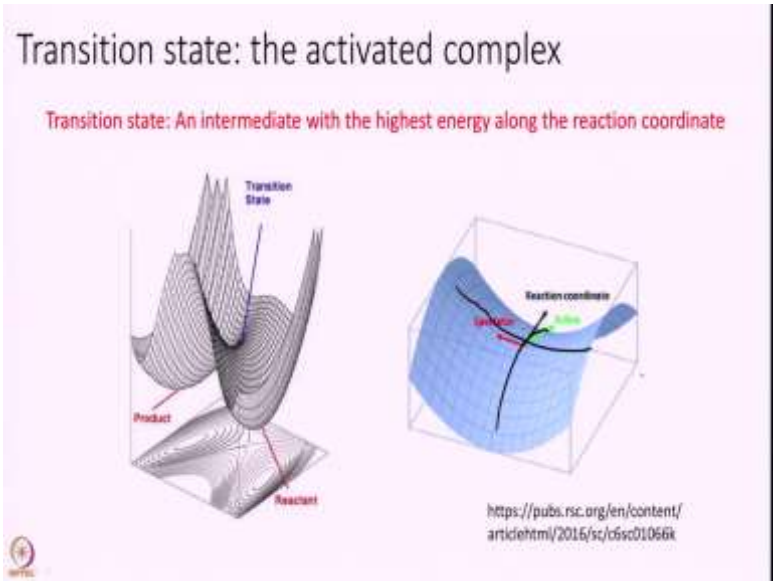

So, let us look at this in terms of a figure here, you see, I have drawn the same thing as my model in terms of a 3D figure. And so, once more the idea is, you have a reactant base in a minima well, you can look at this in the contour plot here, this is my reactant, the product is another base in here, and in between is lives the transition state right here.

So, first the energy has to increase it has to go to transition state and then the energy will go down to become product. And this transition state is again not the minimum energy structure, if I look at a direction, so let us look at closer to the transition state here. I have simply zoomed into the transition states point along the reaction coordinate here.

So, let me get my pen back, this is my reaction coordinate along this line, my energy transition state is the maximum energy structure. But if I draw a line like this, which is perpendicular to the reaction coordinate, then you see that the reaction chord is that the transition state is a minimum energy structure. So that is a very important point you should remember that you should know.

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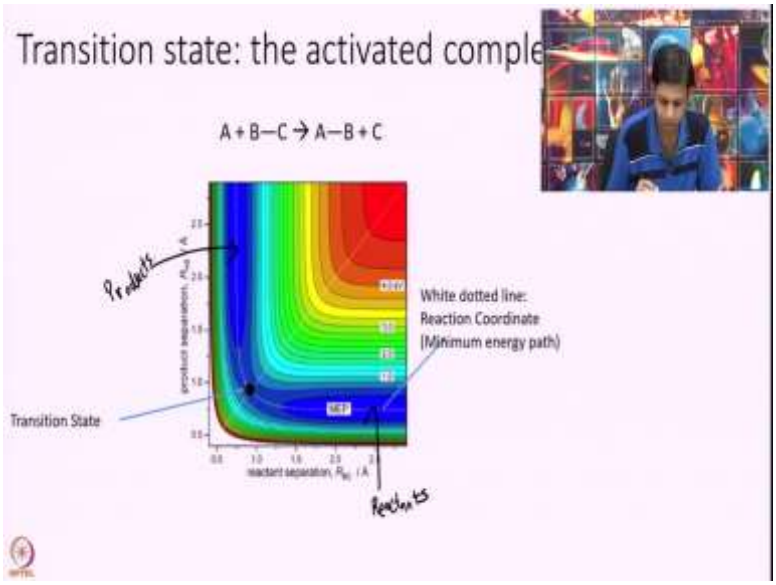

So again, let me re-emphasise this point because it is so important. I have simply drawn a contour plot for a simple reaction of A plus BC going to AB, plus C. This kind of reaction. So, I have RBC coordinate here and RAB coordinate here and I have again the reactants living here this is reactants, this is products and this point is my transition state, this point in the centre here.

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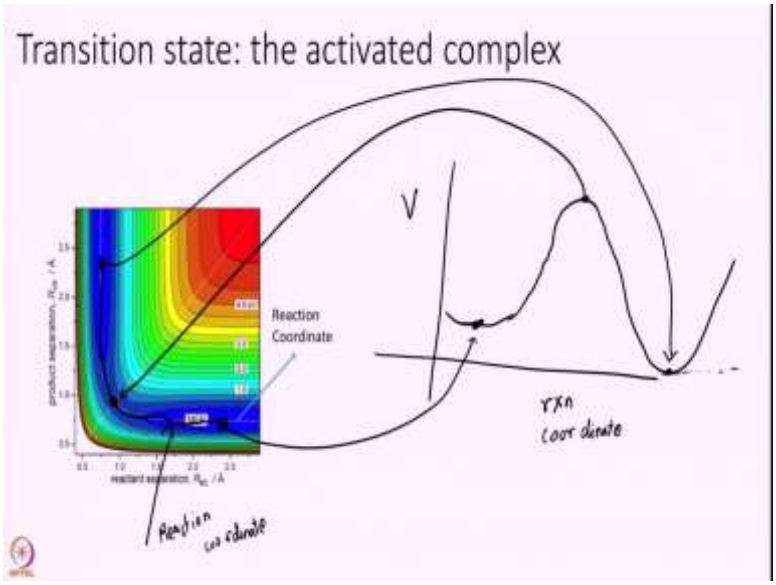

So, let us just be more careful about this let us draw two lines the line that is sorry, the line which is called a reaction coordinate essentially connects that reactant with the transition state with the product, this is called the reaction coordinate. So, if I draw my potential a 1D

potential along the reaction coordinate then what you will get when I am reactant you are getting some kind of a minima here.

So, this point corresponds to this my energy increases to transition state, this point is the same as this point and eventually it decreases like this, this point is the same as this point, in this potential it is not really decreasing like this it probably looks like this that does not matter, it goes from a minima to a maxima to again a minima that is what is important. However, so this figure you must have seen many many times in your high school books. This is always what we show let us also look in another direction.

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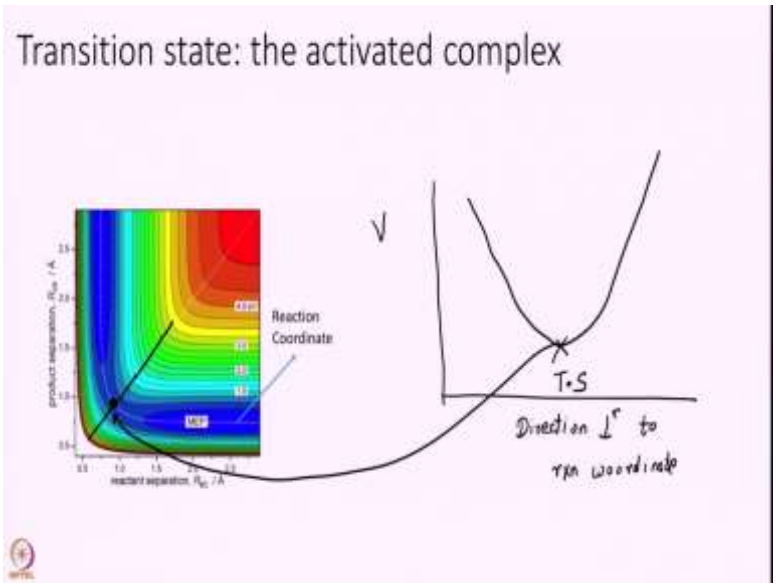

So, let us look at this direction now, why are we only looking at reaction coordinate, why are we so biased. So, let us look at a direction perpendicular to my reaction coordinate. And let us draw my potential here; what do you notice that the transition state here is a minimum energy point. So, you will get potential that will typically look like this. And this point is the transition state. This is the point that connects here.

So, this is very important to know. And this is critical in understanding transition state theory. So, that is all for today. This is one point that I really want you to understand. And that is the reason I am spending this whole module, small, but very important on how to understand this transition state.

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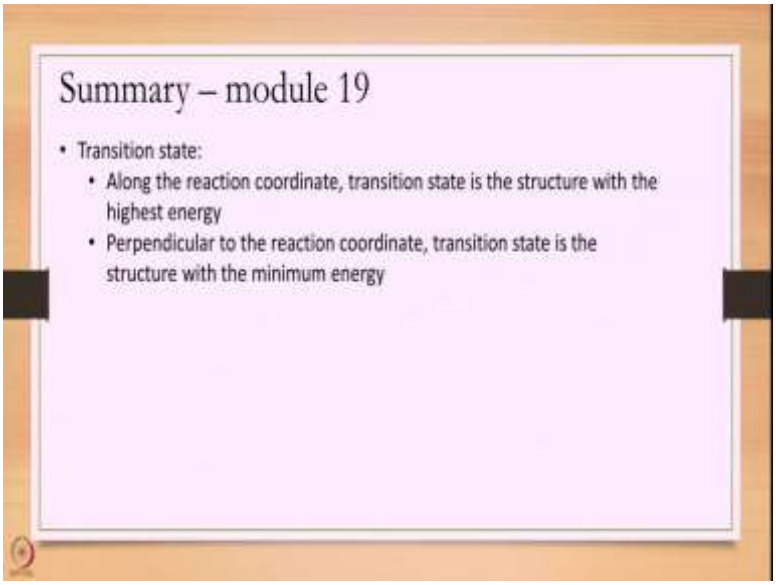

Transition state is the maximum energy structure along the reaction coordinate. Reaction coordinate again, is the part that connects the reactions that connects our reactants to transition state to products. And transition state is also the minimum energy structure along all directions perpendicular to the reaction coordinate. So, the next time, we will formally derive an expression for the transition state theory, building over this concept, and what we have learned in the last few modules about partition functions. Thank you very much.