Rate Processes

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Module No. # 01
Lecture No. # 31

Reaction Dynamics

Good morning everybody. Today, we are back with rate processes and today we will start with reaction dynamics.

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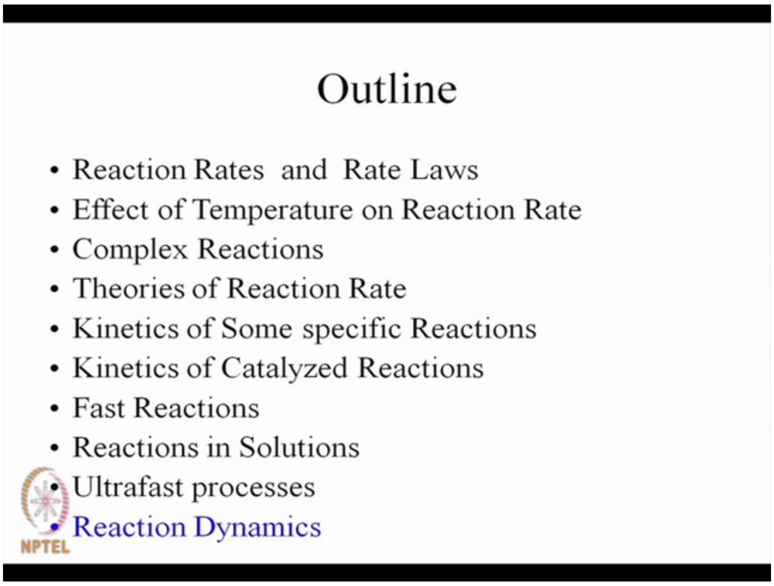

Outline

- Reaction Rates and Rate Laws
- Effect of Temperature on Reaction Rate
- Complex Reactions
- Theories of Reaction Rate
- Kinetics of Some specific Reactions
- Kinetics of Catalyzed Reactions
- Fast Reactions
- Reactions in Solutions
- Ultrafast processes
- Reaction Dynamics

Now, so far we have read, let us see what we have read throughout the series of lectures. We have studied reaction rates and basic rate laws, then effect of temperature on reaction rate, then reaction rate complex reactions, then theories of reaction rates, then we talked about this kinetics of some specific reactions, then kinetics of catalyzed reactions, we talked about fast reactions, reactions in solution. In last few lectures we discussed, we have given outline and just a brief idea of ultrafast processes.

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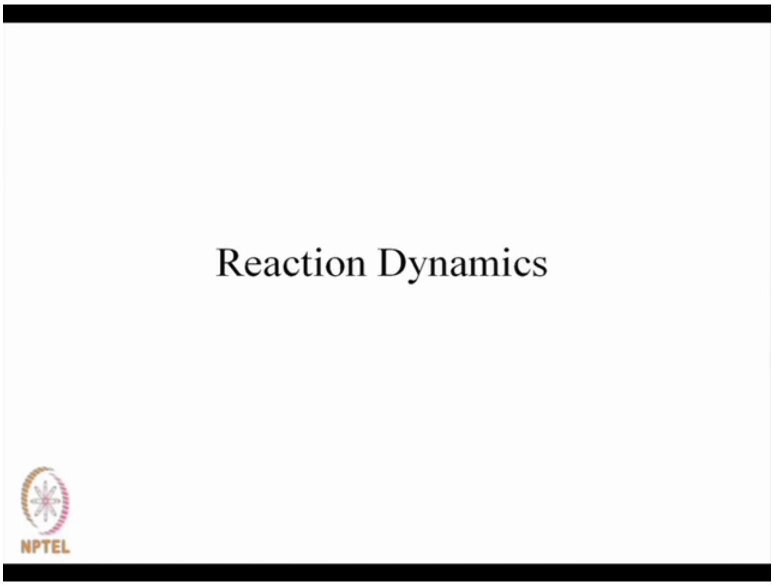

Reaction Dynamics

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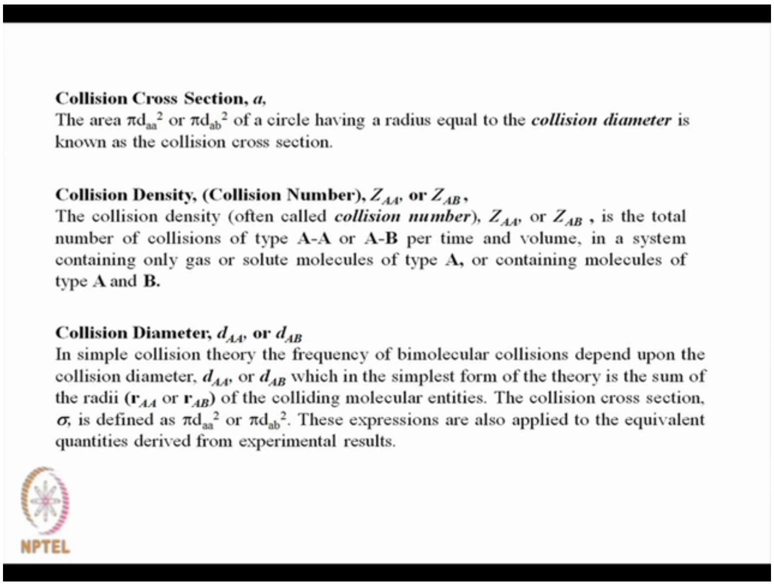

Collision Cross Section, a,
The area πd_{aa}^2 or πd_{ab}^2 of a circle having a radius equal to the ***collision diameter*** is known as the collision cross section.

Collision Density, (Collision Number), Z_{AA}, or Z_{AB} ,
The collision density (often called ***collision number***), Z_{AA}, or Z_{AB} , is the total number of collisions of type **A-A** or **A-B** per time and volume, in a system containing only gas or solute molecules of type **A,** or containing molecules of type **A** and **B.**

Collision Diameter, d_{AA}, or d_{AB}
In simple collision theory the frequency of bimolecular collisions depend upon the collision diameter, d_{AA}, or d_{AB} which in the simplest form of the theory is the sum of the radii ($\mathbf{r}_{AA}$ or $\mathbf{r}_{AB}$) of the colliding molecular entities. The collision cross section, σ, is defined as πd_{aa}^2 or πd_{ab}^2. These expressions are also applied to the equivalent quantities derived from experimental results.

Now we are here with reaction dynamics. Before we start with this, we would like to recap few points before going into the details of the subject.

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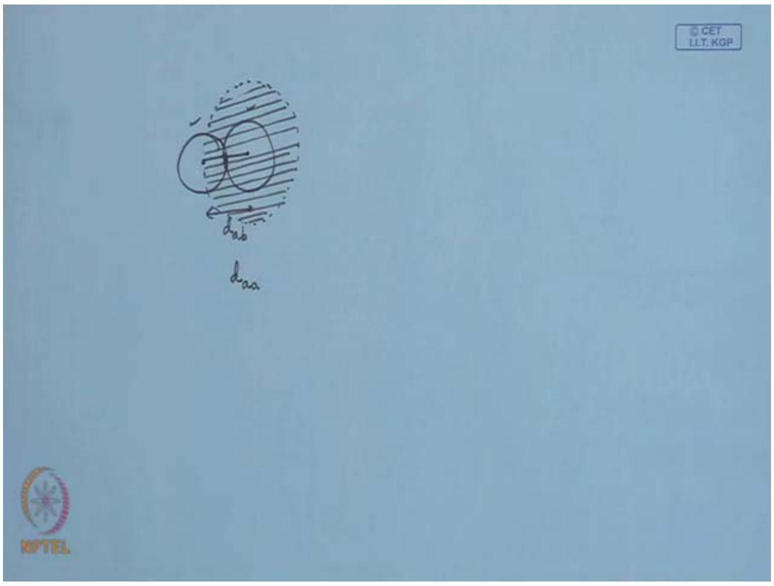

Now, few terms are will be important here. Now one is collision cross section, which is the area that is pi d aa square or pi d ab square of a circle having the radius equal to the collision diameter is known as the collision cross section. So, this is a and say this is b, it is little bit bigger. So, a b a this is d ab or may be if both are same, then it will be d aa.

So, if you draw a circle of this type, then area will be pi d ab square. So, area of the circle having the radius equal to the collision diameter is known as the collision cross section. So, this is your collision cross section.

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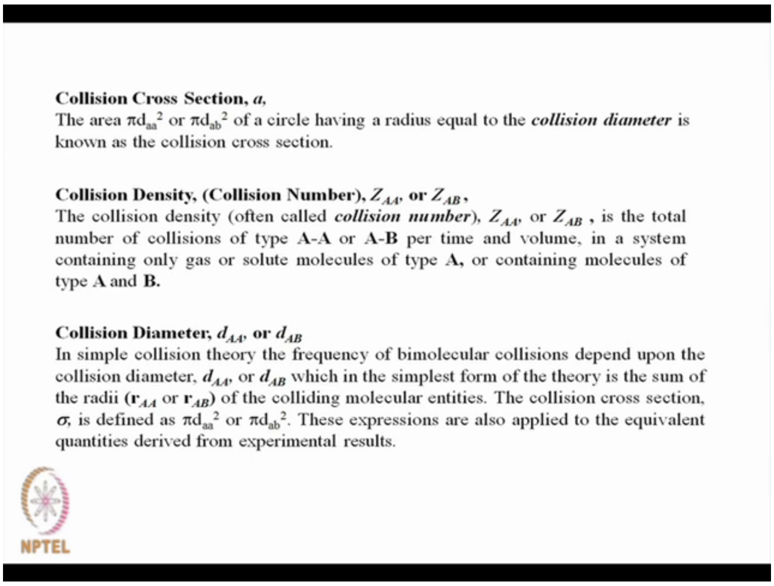

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Then another term collision density or collision number, it is capital Z AA or capital Z AB. This is your collision density, which is often called collision number Z AA or Z AB, is the total number of collisions of type A A or A B per unit time per unit volume in a system containing only gas or solid molecules of type A or containing molecules of type A and B. So, collision density is often called as collision number, which is nothing but the total number of collisions of type A A, that is say A A molecule, collision like this, or A B molecule. So it is the total number of collision per unit time per unit volume in a system containing gas or may be solute of only type or may be containing A and B together. So it is the total number collision remember, it is the total number of collisions of type A A or A B per unit time per unit volume.

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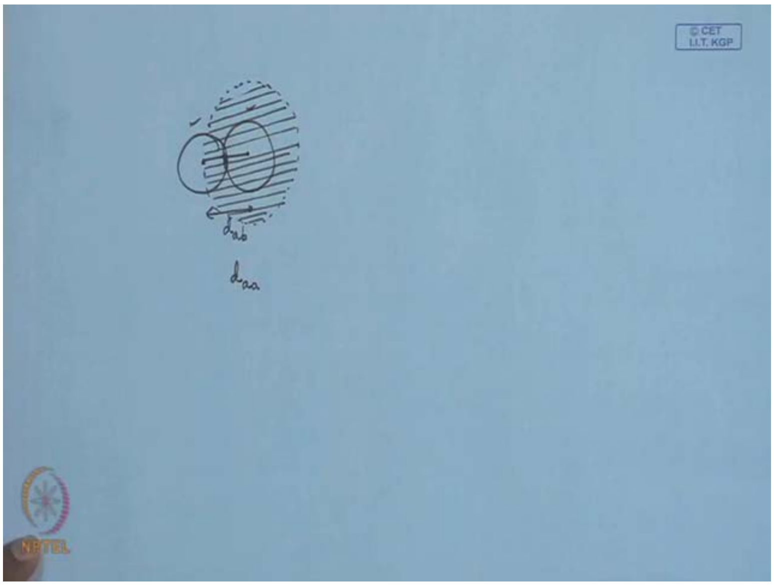

Then collision diameter d AA or d AB, in simple collision theory, the frequency of bimolecular collision depends upon the collision diameter d AA and d AB which in the simplest form of the theory is the sum of the radii r AA or r AB of the colliding molecules, as I told over here. Sum of the radii this radii and the other radii

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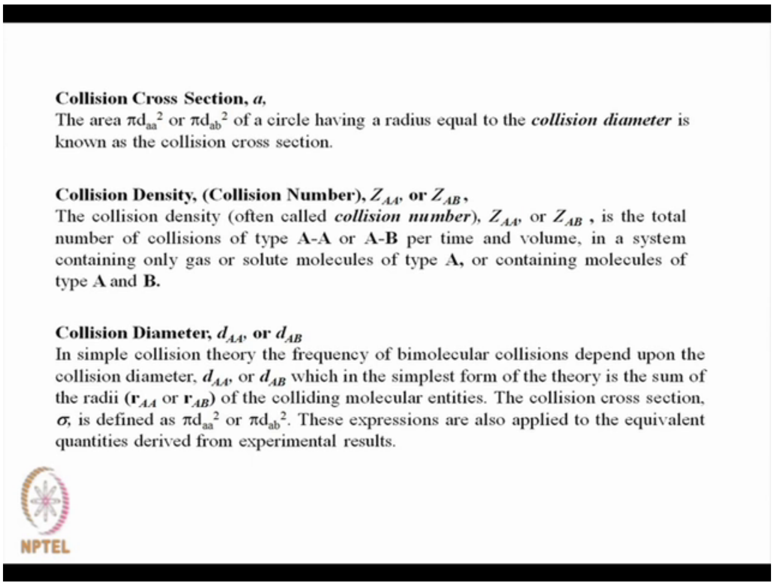

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The collision cross section sigma is defined as, like I already told, it is pi d aa or pi d ab square. These expressions are also apply to equivalent quantities derived from the experimental results. Therefore, collision diameter collision cross sections they are connect by a factor pi d aa square or pi d ab square and d AA and d AB are the collision diameter.

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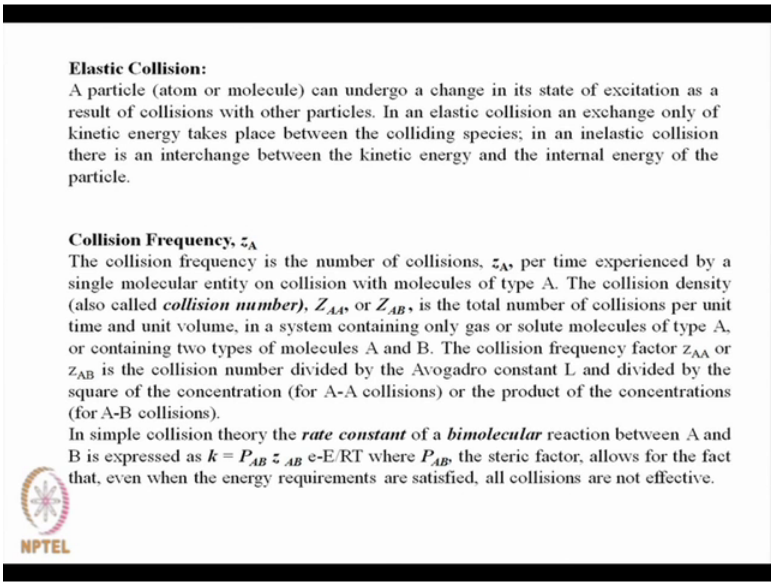

Elastic Collision:
A particle (atom or molecule) can undergo a change in its state of excitation as a result of collisions with other particles. In an elastic collision an exchange only of kinetic energy takes place between the colliding species; in an inelastic collision there is an interchange between the kinetic energy and the internal energy of the particle.

Collision Frequency, z_A
The collision frequency is the number of collisions, z_A, per time experienced by a single molecular entity on collision with molecules of type A. The collision density (also called ***collision number***), Z_{AA}, or Z_{AB}, is the total number of collisions per unit time and unit volume, in a system containing only gas or solute molecules of type A, or containing two types of molecules A and B. The collision frequency factor z_{AA} or z_{AB} is the collision number divided by the Avogadro constant L and divided by the square of the concentration (for A-A collisions) or the product of the concentrations (for A-B collisions).
In simple collision theory the ***rate constant*** of a ***bimolecular*** reaction between A and B is expressed as $k = P_{AB}\, z_{AB}$ e-E/RT where P_{AB}, the steric factor, allows for the fact that, even when the energy requirements are satisfied, all collisions are not effective.

Elastic collision, a particle that is an atom or a molecule can undergo a change in its state of excitation as a result of collisions with other particle. State of excitation means, suppose, because of collision say, this molecule was in the ground just say and say this molecule, this molecule is in the excited state. So when they collide may be, because of energy transfer, the energy of this can be transferred to this. So if that energy is absorbed by this black one, then it may be excited so its state may get changed.

So, its state of excitation as a result of collision with other particle may undergo change. In an elastic collision an exchange only of the kinetic energy takes place between the colliding species, so there is a kinetic energy exchange and in an inelastic collision there is an interchange between the kinetic energy and the internal energy of the particle, so some portion of the kinetic energy has been converted to the internal energy because of some internal arrangement.

So internal energy change means something else, it is not exactly this kinetics case that kinetic energy that initially it was static say, a molecule is hitting then it become static and then it goes away, so it is just change of translational kinetic energy. So inelastic and elastic collisions are different.

Collision frequency small z A, the collision frequency is the number of collisions Z A per unit time experience by a single molecular entity on collision with molecules of type A and collision density capital Z AA or Z AB is the total number of collisions per unit time per unit volume in a system containing only gas or solute molecules of type A or containing two types of molecules A and B.

The collision frequency factor small z AA or small z AB is the collision number divided by Avogadro constant L and divided by the square of the concentration or the product square of the concentration for A collision or the product of the concentration for A B collision. So square for A A and product of the concentrations for A B collision.

In simple collision theory the rate constant of a bimolecular reaction between A and B is expressed as rate constant k is p AB, then small z AB, that is the collision frequency factor then e to the power minus E by RT, where caps P AB is the steric factor allows the fact that even when energy requirements are satisfied all the collisions are not effective.

Suppose, for exchange of atom may be, in this direction along this axis, if that is the requirement and suppose, collision occurs in this way then exchange is not possible, so this collision will be ineffective but this collision will be effective. It is the steric factor that allows the fact that even when energy requirements are not satisfied all collisions are not effective. So steric requirement specific orientational requirement is important.

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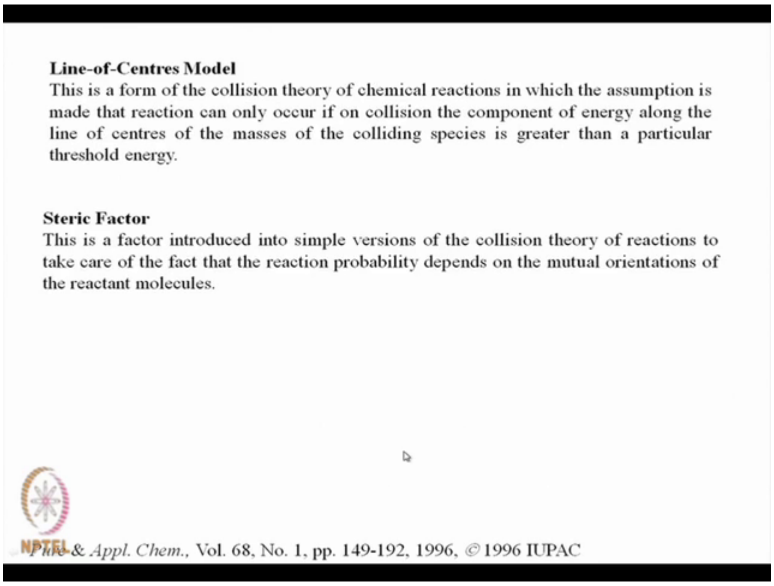

Line-of-Centres Model

This is a form of the collision theory of chemical reactions in which the assumption is made that reaction can only occur if on collision the component of energy along the line of centres of the masses of the colliding species is greater than a particular threshold energy.

Steric Factor

This is a factor introduced into simple versions of the collision theory of reactions to take care of the fact that the reaction probability depends on the mutual orientations of the reactant molecules.

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Line of centres model, this is a form of the collision theory of chemical reactions in which the assumptions is made that the reaction can only occur if on collision the component of energy along the line of centres of masses of colliding particles is greater than a particular threshold energy, and another thing is important which is called the steric factor and this is the factor introduced into a simple version of collision theory of reaction to take care of the fact that reaction probability depends on the mutual orientation of the reactant molecule, as I mentioned over here that a specific orientation is needed, not all orientations are effective in giving chemical reaction product.

So, these are some points that we may be encountering. So, that I just told you so these are taken from pure and applied chemistry this volume and it is the copy right of IUPAC.

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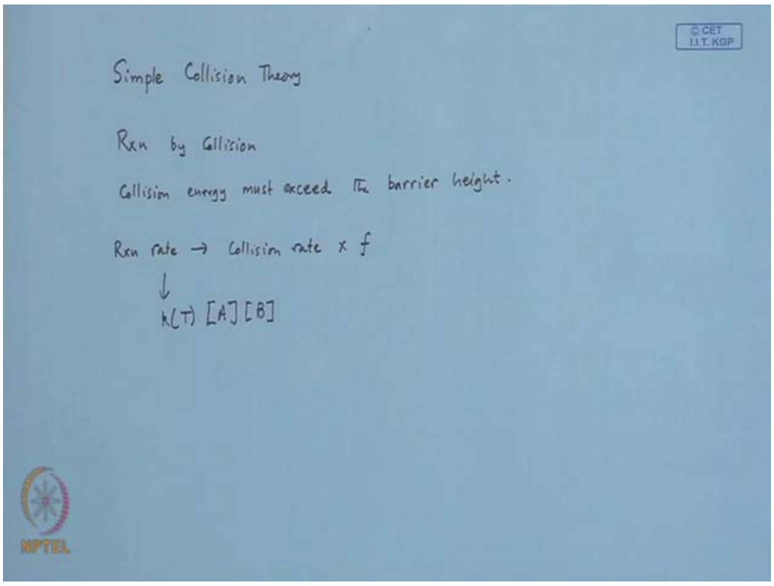

Simple Collision Theory

Rxn by Collision

Collision energy must exceed the barrier height.

Rxn rate $\rightarrow$ Collision rate $\times f$

$\downarrow$

$k(T)\,[A]\,[B]$

So, let us recap the collision theory again, that simple collision theory, the reaction occurs by collision and collision energy must exceed the barrier height, so the reaction rate can be written as collision rate and fraction of collisions times factor f, which represents the fraction of collisions with energy exceeding the barrier height that is e 0.

So, the reaction rate is written as normally reaction rate is written as k, which is the function of times say, concentration of A into concentration. It is a normal way of writing from the chemical kinetics point of view and your collision rate is basically capital Z AB into Z AB into A into B concentration of A into concentration of B.

This is the starting point of our discussion that we will start with simple collision theory, then we will progressively move to the other models.

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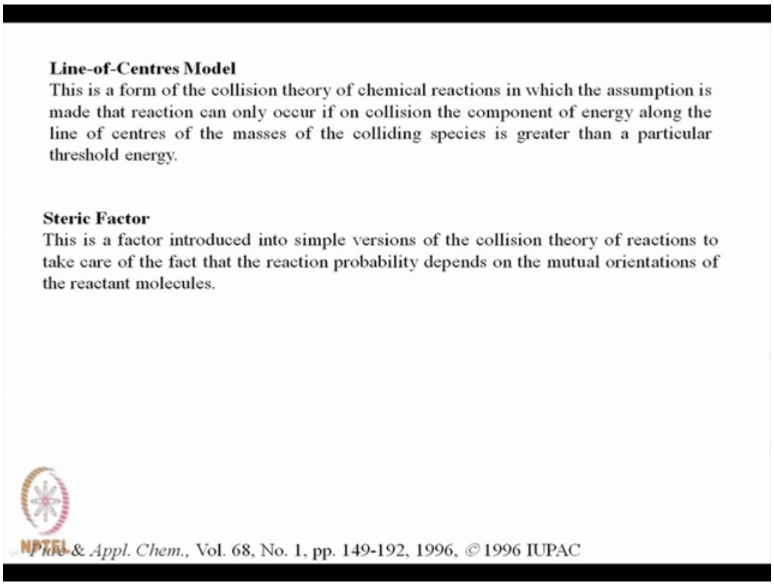

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Now, what is the need for studying reaction dynamics? Now, chemical reaction, why chemical reaction occurs? Chemical reaction has got a connection with chemical reactivity. Chemical reactivity means how reactive the substance is, the substance may be highly reactive may be less reactive.

So, reaction dynamics has got this thing that understanding of means, it tries to relate some aspects of chemical reactivity that is aspects like understanding of chemical reactivity, predicting and also controlling. So how can you control reactivity? how can you predict that this reaction predict about the reaction? and also it gives us understanding of chemical reactivity.

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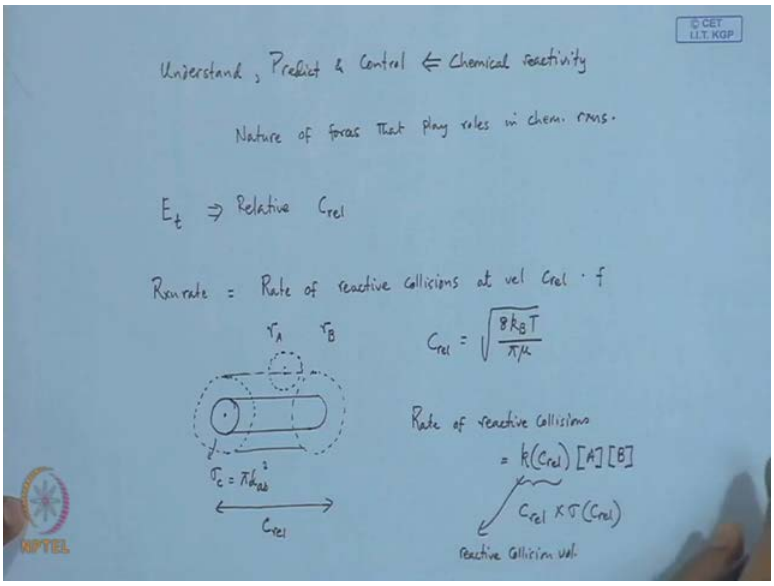

Understand, Predict & Control ⇐ Chemical reactivity

Nature of forces that play roles in chem. rxns.

$E_t \Rightarrow$ Relative c_{rel}

Rxn rate = Rate of reactive collisions at vel $c_{rel} \cdot f$

$c_{rel} = \sqrt{\frac{8 k_B T}{\pi \mu}}$

Rate of reactive collisions

$= \underbrace{k(c_{rel})}_{c_{rel} \times \sigma(c_{rel})} [A][B]$

reactive collision vol.

Now, we will be curious to know about the nature of forces that play in chemical reaction. So the thing is that chemical reactivity we wanted so reaction dynamics has got the connection like we wanted to understand, predict and control chemical reactivity and we are curious to know the nature of forces that are there.

So, we also would be happy to know the nature of forces, that play crucial role in chemical reaction and also when it is the question of chemical reaction that is, as I told you, that a minimum amount of energy must be there to cross the barrier, that is all collisions are not effective.

Certain collisions with having energy greater than the barrier height can cross the barrier and lead to products, so when it is the question of barrier then naturally, question of potential energy surface comes. So, we would I like to know the nature of potential energy surface as well.

So, the principle idea is that, the basic idea is that the reaction occurs by collision and collision energy must exceed the barrier height otherwise, it will not cross the barrier. So it is an activated barrier crossing process. You have got your reactant and you have got your product.

So, it will not come directly from here to here, from here to it will not come directly so, it will come via a barrier to here. Now, when collision energy is say, given by a quantity say, E t and if that corresponds to a relative velocity, relative velocity between the colliding entities like this. So relative velocity if that corresponds to, I mean, that is written like C relative.

Then reaction rate can be written as rate of reactive collision, because collision rate will determine the rate of reaction. So rate of reactive collision, those collisions which are reactive not all collisions give rise to product.

The rate of reactive collisions at velocity C relative into the fraction of collision that are effective into f. Now let us draw I mean, which one is I mean, when there is a there is a question of collision then may be, in some cases they will collide in some cases they will just touch or may be, just miss or may be, a true miss so this is your one atom and of course this is the idea is that, here we have to think that these reactants are rather structured, they do not have any specific structure may be, like a hard sphere and reactants are having radii r A and r B.

So, basically what is happening that it is like, you have to draw a cross section so and you draw a cylinder like this also, so if your second molecular second atom I mean the reactant is here I mean, its centre is either here or inside then, there will be a collision but if it is just outside then it is just miss. So those basically, if it is like this, second structure less entry so it this will not hit. There is a difference.

So, that means this collision cross section is sigma c which is equal to pi d ab square and this is relative speed so that, means this length is nothing but C rel and this C rel is equal to at given temperature, it is square root of 8 k B T by pi mu where mu is the reduce mass of the system that is m a and m b. So, rate of reactive collisions, you can write in this way rate of reactive collisions equal to some k designated at I mean, C rel, concentration of A and concentration of B

So, now, k C relative, this is number of reactive collision which is nothing but k C relative, which defines the reactive collision volume swept out per unit area. So k C relative is nothing but your C relative into sigma. So this corresponds to the reactive collision volume, where this is the collision cross section characterized by C relative I mean, at C relative.

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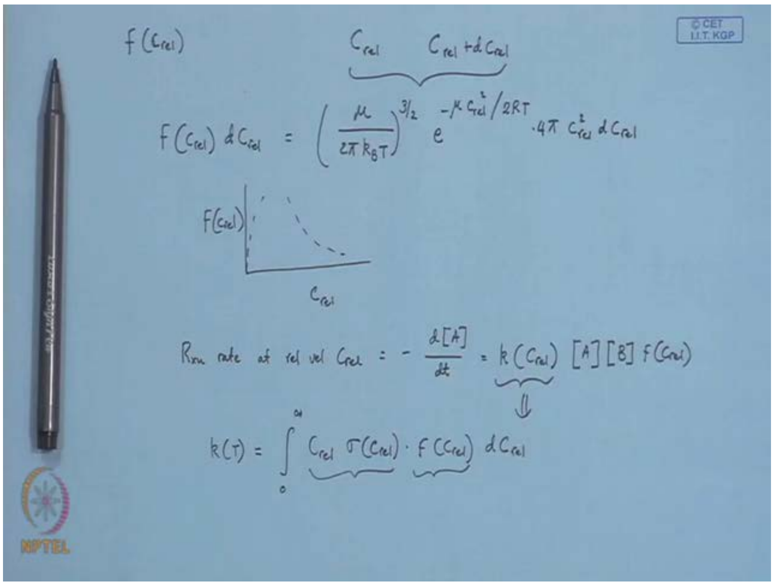

$f(C_{rel})$ $\qquad \underbrace{C_{rel} \qquad C_{rel} + dC_{rel}}$

$$f(C_{rel})\, dC_{rel} = \left(\frac{\mu}{2\pi k_B T}\right)^{3/2} e^{-\mu C_{rel}^2/2RT} \cdot 4\pi C_{rel}^2\, dC_{rel}$$

$$\text{Rxn rate at rel vel } C_{rel} : -\frac{d[A]}{dt} = \underbrace{k(C_{rel})}_{\Downarrow} [A][B]\, f(C_{rel})$$

$$k(T) = \int_0^\infty \underbrace{C_{rel}\, \sigma(C_{rel})} \cdot \underbrace{f(C_{rel})}\, dC_{rel}$$

Now, next comes the point that f c relative. f C relative I mean, there is a fraction we define another quantity f C relative is fraction of collision with velocities in the range C relative and C plus d C relative that is, if the velocity lies in the range C and C plus d C of course, C relative and C plus d C relative so. C relative and C relative plus d C relative. We just would like to know what is the fraction of molecules or what is the fraction of collision in this relative speed range that we wanted to know.

So, in that case we have to use the Maxwell's velocity distribution that, f C relative d C relative which is equal to mu by 2 pi k B T to the power 3 by 2, it is a three dimensional case that is why it is 3 by 2, e to the power minus mu C relative square by 2 RT into 4 pi C square relative d C relative and it has got if you plot, it will be something like this. This is your C relative and it is f C relative.

Therefore, actual reaction rate when relative velocity is C relative is given by reaction rate at relative velocity C rel is given by minus d A dt is equal to k C relative into B into f C relative.

So, this is basically your reactive collision volume. The thermal rate constant is obtained by averaging this one which is nothing but C relative and sigma C relative and over and that has to be averaged over Maxwell Boltzmann distribution therefore, average k T can be written as integration from 0 to infinity, that is we are integrating for all the speeds.

C relative into sigma C relative into f C relative d C relative. So this is your probability function, this is your quantity and this is the integration variable. So that will give you the thermal average k T and of course, the denominator should have a normalizing constant so and generally normalization constant, we do not try because it is taken to be normalized to one so that is why we do not try the normalization constant in the denominator, so it is the expression for the thermal average rate constant.

Why thermal average? Because it has to be averaged over C relative because, there are number of relative velocities I mean, not all relative velocities are effective, so this relative velocity will range from 0 to infinity and temperature means, it is a measure of mean random translation of kinetic energy so, it is a randomly distributed and this kinetic energy it is random thing therefore, we have to think of all the possibilities and we have to integrate over the entire range of C and this is your probability function that is, probability of having a speed from value C to C plus d C is given by this. So this probability takes care of the fact that which speed is most probable which speed is less probable and so on so that is why it is a right average quantity.

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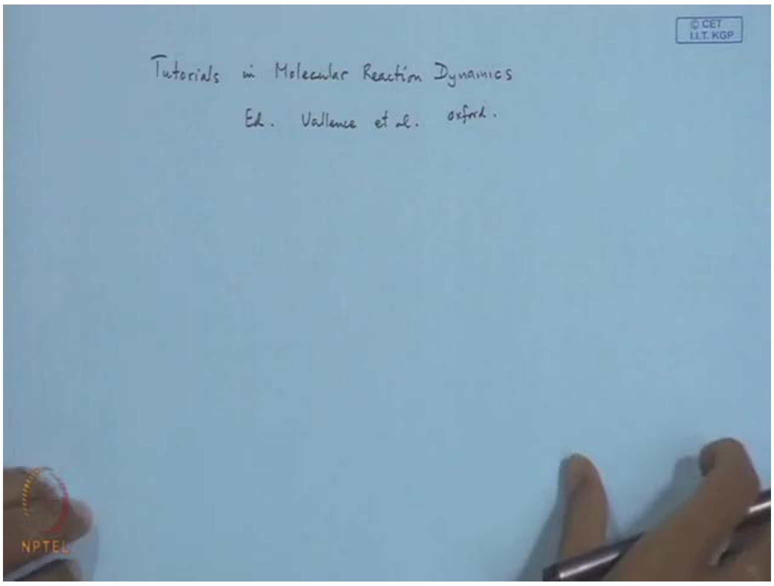

Tutorials in Molecular Reaction Dynamics

Ed. Vallence et al. oxford.

Next we will see some, we would like to talk on some state resolved properties. Before that, for this particular topic let me give some references like book by Raphael D Levine and other books I already shown in the first few lectures plus another book by tutorials in molecular reaction dynamics edited by Valence and another author. It is available in oxford. So, that you can consult for this particular piece of topic that reaction dynamics in addition to this book by Raphael D Levine and other books I referred earlier.

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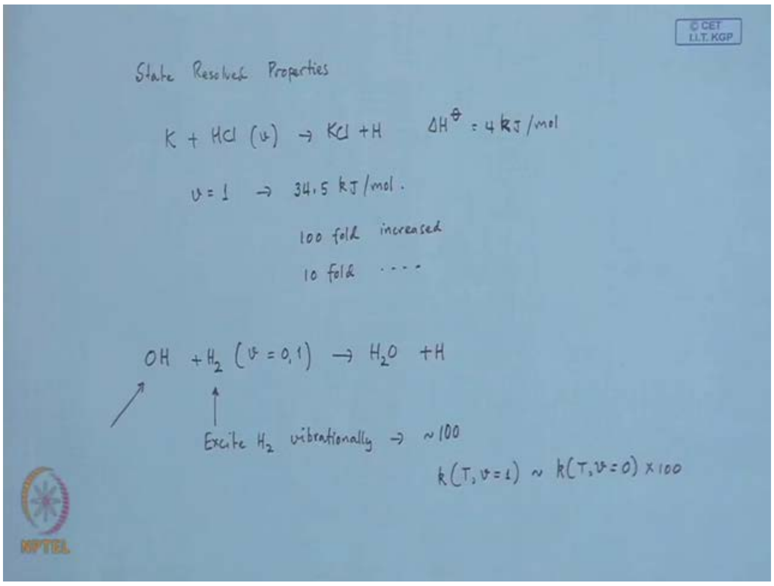

State Resolved Properties

$K + HCl\ (v) \rightarrow KCl + H \quad \Delta H^{\ominus} = 4\ kJ/mol$

$v = 1 \rightarrow 34.5\ kJ/mol.$

100 fold increased

10 fold ....

$OH + H_2\ (v = 0, 1) \rightarrow H_2O + H$

Excite H_2 vibrationally $\rightarrow \sim 100$

$k(T, v=1) \sim k(T, v=0) \times 100$

Now state resolved properties, now let us consider one reaction K plus Hcl in the vth vibrational level gives rise to Kcl plus H or standard enthalpy delta H 0 bar is 4 kilo joule mol inverse and when v is equal to 1 for Hcl the corresponding energy is 34.5 kilo joule per mol.

Now, if you put this energy to Hcl thereby, giving rise to vibrationally excited to generate the vibrationally excited Hcl, then it has been found that rate is increased that is rate is 100 fold increased but, if you put this energy to the translational degree of freedom then the rate has been found to be 10 fold increase.

So, what can you say about it means, what is the conclusion that vibrational energies for the reaction to occur that vibrational energies are more important than the translational efficient I mean, vibrational energies are more efficient in promoting chemical reaction than translational energy so you can recall one thing that, this theory of absolute reaction rate that when reaction occurs then one bond is say formed and another bond is broken so the bond which is broken is required to undergo a low frequency large amplitude vibration, so that particular low frequency vibration is converted to translation.

From this example, you can think of that vibrational energy could be more important and of course it is 100 fold increased and one in another case 10 fold. So vibrational energies are more efficient in promoting the reaction than does translational energy, that is you supply energy to translational mode reaction it increases, I mean, collision are more but may be if you supply to the vibrational degrees of freedom may be, it is increased more that is if you increase the energy to the internal moods like, now the translational, I mean vibrational mode then it happens.

Another example, hydroxide radical plus H2, v is equal to 0 1 giving rise to H2O plus hydrogen. If you excite vibrationally this hydrogen, excite hydrogen vibrationally, then rate constant has been found to increase by a factor of 100, which is basically k T. v is equal to 1 is of the order of k T. v is equal to 0 into 100. But if you excite this spectator I mean, this which vibrationally then it has got it does not have that much of effect.

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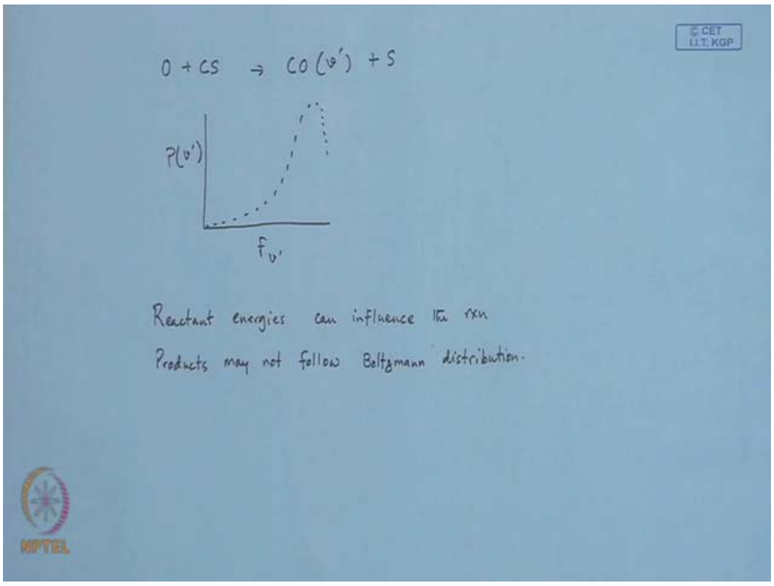

$O + CS \rightarrow CO(v') + S$

Reactant energies can influence the rxn

Products may not follow Boltzmann distribution.

Again it says, that vibrational excitation is sometimes is very efficient in promoting the chemical reaction. Now, think about another reaction, that another example O plus CS giving rise to CO different vibrational level plus S and if you plot probability v prime and a come and F v prime then may be it maximizes at some higher value. So there is a population inversion in carbon monoxide vibrational level, that is, your product is carbon monoxide, so there is a population inversion which is not designable at ordinary temperature, so that is, ordinary temperature says that, says Boltzmann, population that if the higher level is there and if the energy gap is more than thermal energy that is k T then, population will be less, that is, lower levels will be populated more compared to the higher levels so in that case, the system is not under thermal equilibrium.

So, reactant energies can influence the course of reaction and the products which are form that may not follow the Boltzmann distribution, products may not follow Boltzmann distribution and we would need to prove the population, prove the population over the product states and control the populations in the reactant states.

For example, one thing is important that velocity, that is, important thing is it is magnitude and direction and vibrational rotational energies, these are nothing but the internal degrees of freedom so that is, important to orientation factor that is another important thing.

Now the examples which we cited like three examples over here clearly demonstrates that reaction cross section is dependent on velocities of your reactants, then, the vibrational and rotational states of few reactant and also may be the orientation is very important, so that part will be coming to later on, so vibrational rotational state and this velocities with which it is colliding is very important.

Next, we have to think of, when it is the question of collision between two entities having no specific structure may be, two balls are colliding. So the collision may be elastic collision, may be inelastic, so we have to think of the conversation because you know, somehow it will be conserved may be, if the collision is not elastic so some means energy may be transferred in some other degrees of freedom or in some other way may be in the form of heat or else. Now consider reaction like A plus this giving rise to A B plus C.

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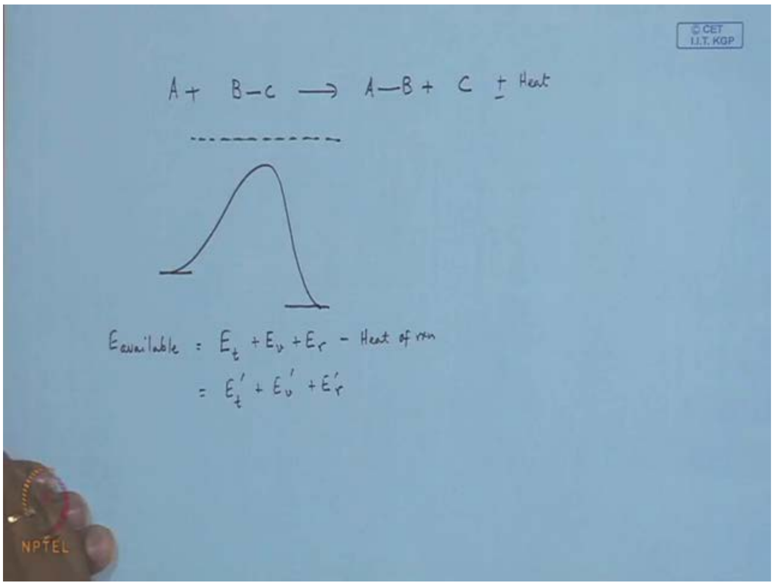

$A + B-C \longrightarrow A-B + C \pm \text{Heat}$

$E_{\text{available}} = E_t + E_v + E_r - \text{Heat of rxn}$

$= E_t' + E_v' + E_r'$

Now, conservation of energy says that, the energy which is available now for a particular reaction, suppose, you have got your reactant over here and may be product over here, and it is going from reactant to product this way. So this is the total energy. So, available energy you can write in terms of, E available is E total plus I mean, E translation plus E vibration plus E rotation minus heat of reaction I mean, enthalpy of reaction. So basically this heat of reaction you can write in this fashion may be, this energy may be, if it is distributed over here then may be E prime translation plus E primed vibration plus E primed rotation.

So, the because of this process from a to b so, energy must becomes up that is, this side energy and that side energy must becomes up plus something may be plus minus heat. So, if you add up here, if you add up here then it must be comes up, so conservation of energy, it is very important for such process to occur and it may be may be computed either in terms of reactants or in terms of products.

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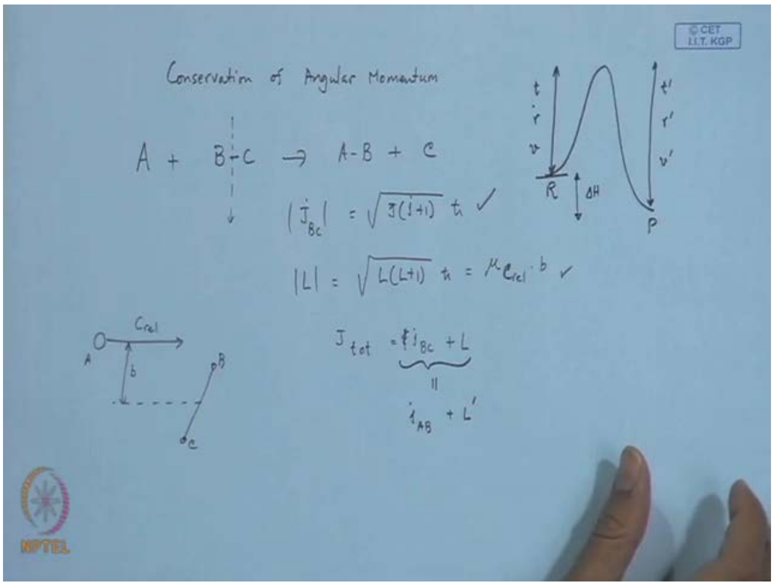

Conservation of Angular Momentum

$$A + B-C \rightarrow A-B + C$$

$$|\dot{J}_{BC}| = \sqrt{J(J+1)}\,\hbar \checkmark$$

$$|L| = \sqrt{L(L+1)}\,\hbar = \mu c_{rel} \cdot b \checkmark$$

$$J_{tot} = \underbrace{j_{BC} + L}_{\parallel}$$

$$j_{AB} + L'$$

Another important thing is that, conservation of other quantities like angular momentum that is also an important thing. So not only energy conservation but also, energy conservation energy it is applicable as also the other conservation principles like, conservation of angular momentum is important. So what about rotation? Now thing is that we are talking about A plus B C giving rise to A B plus C. So this has got the rotational angular momentum, so J BC is equal to root over J into J plus 1 in h plus unit so this has got the angular momentum.

Now, in the same way orbital angular momentum will be given by I mean, total angular momentum is nothing but it is your rotational and orbital angular momentum L will be given by root over L into L plus 1 in h plus unit and which is basically mu into C relative into b, b is the separation between say, you have got your say B this is C and say, this is your A which is coming in this way A with C relative and separation b. So m r I mean, it is basically mu r into rate of velocity so total angular momentum.

So, rotational angular momentum is this and orbital angular momentum is this. So in computing the orbital angular momentum you have to make use of this diagram. So total angular momentum is given by J total is equal to J BC plus L. So this way orbital angular momentum and total angular momentum they can be used in I mean, or orbital angular momentum and your rotational angular momentum can be used over here.

So, and of course, this is your reactant side and for the product side what is happening? That product side it will be corresponding this value will be j AB and plus say, L prime so this two will be equal so conservation of total angular momentum will be there. So this way, we have to consider the conservation of angular momentum.

Like here, in case of your energy, so your reactant side is like this if you think of energy that say, this is your reactant, this is your product so may be, this corresponds to translation, rotation and say, vibration combination and may be this corresponds to say, translation primed, rotation primed and vibration primed. So we have to make use of this equalization and of course this is your heat of reaction. So this is your delta H of the process so this way you can equalize this and that (( )) left hand and right hand side.

So, that is about the conservation laws. So we have to think of the conservation principle. Now, I will stop today and may be, next lecture I will take up the forces and potential energy factors and energy factors various potential energy types, I mean, potential energy carb for diatomic system etcetera. I will take up so what we have learnt today let us have a quick recap.

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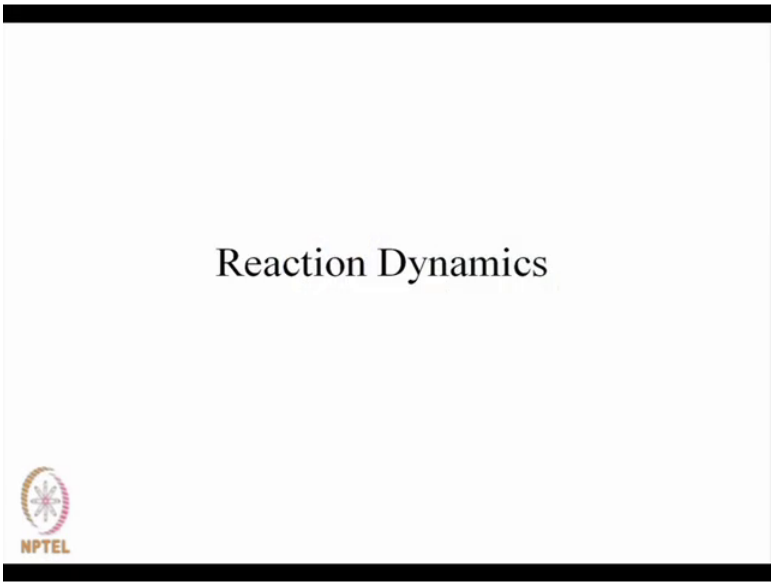

Reaction Dynamics

That we wanted to start with this reaction dynamics to understand the chemical reactivity, to predict chemical reactivity and also controlling chemical reactivity. We would like to know the nature of forces responsible for the, I mean, nature of forces that play roles in chemical reaction and also we would like to know the potential energy diagram which is of a prime importance.

We started with collision theory, collision theory of reaction that collision in gas phase, collisions are responsible for chemical reaction to occur and not all collisions are effective. Certain collisions are ineffective may be energy wise because that is that threshold energy is crossed may be, so collision sometime collision may be not be effective.

So, we gave certain examples, we gave cited certain example that state resolved properties and how vibrational energies are, I mean, vibrational excitations are more efficient than translational excitations and we gave examples on that, then we started with conservation laws. It is the energy conservation must be followed left hand side and right hand side energy conservation must be followed, total energy in the left hand side and total energy in the right hand side that is available energy means total energy of the system translational energy rotational energy vibrational energy in the reactant side and in the product side. So as if this difference in you can think in this way that your reactant side in the left hand side and the product side in the right hand side what is happening that, these are these are connected by delta H, the difference is called delta H so as if, this excess delta H I mean delta H of the reaction is there with your reactant side. The moment it is converted to from reactant to product, this energy which was there is released in terms of heat of reaction.

So, conservation of energy is there and also conservation of angular momentum that is, very important that also has to be improved. So I mean, when there is a gas phase reaction may be may be conservation I mean it is say, this is one species is a and this is b c so, they collide like this. So it has got this your rotational angular momentum and the orbital angular momentum because of this geometry, I mean, a and this b c so, these two together are needed to be considered for applying the conservation.

So, I guess that is all for today. So next lecture will take up this potential energy and energy issues, potential energy carb and those things like attractive potential energy carb or may be the potential energy carb that is for say, may be, this diatomic potential energy carb we will take up that issue and we will proceed further so till then, thank you.