

Hello students, here we are looking  
at course code CHC 104 Course title,  
physical chemistry and inorganic chemistry.

In this module we will be looking

at unit title Chemical Kinetics

and dealing with module name:

concept of activation,

energy and its calculation

from the Arrhenius equation.

I am Miss Priyanka Fernandes,

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College, Cortalim. So in this module,

we will be looking at what is

activation energy and how it

impacts the rate of reaction.

The definition of what is temperature

coefficient and finally the

calculation of activation energy

at two different temperatures.

So students at the end of this module

you will be able to explain the role of

activation energy in reaction rates.

You will be able to give the

Arrhenius equation and define

what is temperature coefficient.

Derive a formula for calculating the

activation energy at two different

temperatures and graphically represent

the same and finally solve problems with

respect to the activation energy formula.

So let us understand how reactions

Proceed. Now according to the concept of

Activation, reactants do not directly

form the products. The reactants first

collide and how do they collide?

They do that by,

absorbing certain minimum amount of energy

that energy is known as activation energy

and then they form their products.

As you can see here in this diagram,

we have two atoms of reactant A

and two atoms of reactant B. Both

these reactants proceed to form a product having two molecules AB.

How does this reaction form?

As you can see,

the reactants need to collide.

After they collide,

they acquire some amount of energy which is greater than the energy barrier.

The yellow line that you see here is the energy barrier.

Now these reactants need to possess the energy greater than the energy barrier in order to proceed to the products.

This energy that they possess on collision is nothing but your activation energy, which is the area under the curve.

So kinetic energy of a gas we all are aware is directly proportional to temperature.

So we can say that as the temperature of a system is increased, more and more molecules will

acquire an excess energy that is greater than the energy barrier in order to cause productive or effective collisions.

This will further increase the rate of a reaction.

Thus,

the minimum amount of energy required for the collision between the molecules to be effective is called as energy of activation.

So, energy of activation depends on the nature of the reactants and eventually we can conclude that those reactions which require high amount of activation energy will be slow reactions while those reactions which require minimum or less amount of activation energy will proceed at a faster rate.

Now, in 1889,

Arrhenius suggested a simple relationship between the rate constant  $K$  of a reaction and the temperature of the system.

So Arrhenius, a great scientist gave the following relationship.

That is,

$K$  is equal to  $Ae$  raised to minus  $E_a$  by  $RT$ .

What are these notations?

Here  $A$  is a frequency factor, which is experimentally determined.

$E_a$  is the activation energy,

$R$  is the gas constant,

which is usually taken as a value

8.314.  $T$  is temperature in Kelvin

and  $e$  is logarithmic base,

which is equal to 2.718.

Now according to Arrhenius,

increasing the temperature by

10 degrees Celsius is said to

double the rate of a reaction.

So suppose now students we consider

two reactions: one occurring

at a lower temperature and the

second reaction occurring at a

10 degrees increased temperature,

we can say that the ratio of the

rate constants in the first case,

the rate constant will be  $k_1$ .

In the second case  $k_2$ .

So here we see these rate constants of the

reaction at two different temperatures,

which are differing by 10 degrees. This is

called as temperature coefficient.

So we can represent temperature

coefficient as the rate of the first

reaction and rate of second reaction.

What we do is, we take the higher value

that is rate of the second reaction,

say occurring at a temperature of 35

degrees Celsius and the first reaction

whose rate constant is at

a temperature of 25 degrees celsius.

Now we need to convert degree Celsius

to Kelvin by adding a value of 273.

And what you will achieve is a rate constant

which is occurring in between

the values ***two and three***.

So how to calculate activation energy

at two different temperatures?

We will be looking at it with a derivation.

So here you invoke the Arrhenius equation

$K = A e^{-E_a/RT}$ .

You take the natural log on

either side of the equation,

both RHS and LHS.

So you get natural log of K is equal

to minus  $E_a$  plus natural log of

the constant  $Ae$ . This you convert

to logarithmic base to the base 10

where you have  $\log K$  is equal to

minus  $E_a$  upon  $2.33 RT \log$ .

So here we are converting the

natural log to log to the base 10

by dividing with a value 2.303.

So at two different temperatures

we can write these two equations.

The first reaction we consider

the rate constant to be  $k_1$ ,

so log of  $k_1$  is equal to minus

$E_a$  upon  $2.303 RT_1$  that is the first temperature

$T_1$  plus log of the constant.

Similarly,

second reaction you can write as log

$k_2$  equal to minus  $E_a$  upon  $2.33 RT_2$  plus log of the constant.

Next,

what we do is we subtract the

smaller value from the bigger value.

So you need to subtract

equation (1) from equation (2).

What you get after that is log

$k_2 \log k_1$  equal to minus  $E_a$  upon

$2.303 RT_2$  plus log 8 minus the

first equation which is minus  $E_a$

upon  $2.303 RT_1$  plus  $\log$  .

On doing so,

we can eliminate certain constants,

so plus  $\log A$  and minus

$\log A$  can be cancelled out

and you are left

with  $\log k_2$  minus  $\log k_1$  equal

to minus  $E_a$  upon  $2.303$  are in

bracket.  $1$  by  $T_1$  --  $1$  by  $T_2$ .

This then on finding the LCM you

can write as  $\log k_2$  minus  $\log$

$k_1$  equal to  $E_a$  upon  $2.303$  into  $T_2 - T_1$  upon one into  $T_2$ ,

here by interchanging the values of

$T_1$  and  $T_2$  we can eliminate the minus

sign before the activation energy.

So finally, we get an equation

where  $\log K_2$  minus  $\log K_1$  can be

written in the form of a numerator

divided by the denominator,

that is  $\log K_2$  by  $K_1$  equal to  $E_a$  upon  $2.303$

$R$  into bracket  $T_2 T_1 / T_1$  into  $T_2$ .

The same equation can be represented in the form of a graph.

Here again, you

invoke Arrhenius equation and this equation

you write down the natural log of it.

That is natural log of K equal to minus

$E_a$  upon  $RT$  plus natural log of A.

Now this equation can be represented in

the form of an equation of a straight line,

which is  $E_a$  equal to  $mx + c$ .

When we do this,

what we get on the Y axis is

natural log of K. On the X axis

You obtain one by T.

Here we can see the intercept is

natural log of A and the slope

can be written as minus  $E_a$  upon R.

So, in general log to the base ten,

we can write the slope m which is

equal to minus  $E_a$  upon  $2.303$  into R.

This value is taken for solving

different word problems.

Now we usually say that one can only

learn a formula by applying it in problems.

So let us now solve a problem.

Here you have a reaction given to you,

which is a gas phase reaction

between methane and sulfur.

Now it is said that at 550 degrees Celsius

the rate constant for the reaction

is given as 1.1 mole litre inverse.

At however,

625 degree Celsius the rate

constant becomes 6.41 mole litre inverse.

You need to calculate

the activation energy of the reaction.

So let us use the formula here.

Before that we need to write

what is given to us.

So gas constant we are aware of is

8.314. Temperature 1 is given as 550

degrees Celsius to which we need

to add a value of 273 to convert

it into the Kelvin scale. Rate

constant of the first reaction

is given to you as 1.1.

Similarly,

the second temperature is given as

625 degrees Celsius on converting

to Kelvin you get the value as

898 Kelvin and the rate constant

of the second reaction is 6.41.

So you can write this equation that we

have just studied on putting in the values.

This is what we get, 0.76 which is equal

to  $E_a$  upon  $19.14$  into bracket  $1.1$  into  $10$ ,

raised to minus four.

So what we do is keep the unknown

value on one side and take the

known values on the other side and

multiply and divide accordingly.

On doing so we get the final answer as

$1.4$  into  $10$  raised to five Joule per mole,

which is the final activation energy.

Let us look at another problem here.

The rate constant of a reaction at 20

degrees Celsius is known to be half of

the rate constant at 30 degrees Celsius.

You need to calculate the energy

of activation of the reaction.

Here the value of R is given

to you in the form of calorie

kelvin inverse mole inverse which is 1.987

Now see students.

First, we write the equation

and here we can do

one thing is assume the rate constant.

So it is said that the rate constant of this

second reaction is double the first reaction.

Or in other words rate constant of

first is half of the second reaction.

So we can easily assume rate

constant of second reaction to be 2.

Hence the rate constant of

first reaction will be one.

If you divide  $k_2$  by  $k_1$  you will

get 2 by 1 which is 2 itself.

You write the value of  $R$ ,

which is given to you and next you need to

put in the values in the Arrhenius equation.

So temperature as well

you need to mention in terms of Kelvin.

On putting in the values,

what you finally get is an answer 12228.36

calories which is activation energy.

Now this calorie you can convert

into more appropriate form,

that is kilo calorie.

The answer is divided by 1000.

On doing so you shift the decimal point and

get a final answer of 12.22836 kilo calorie,

your final answer for the activation energy.

So as a summary what we have

seen is that activation energy is the

minimum quantity of energy which the

reacting species must possess in order  
to undergo a specified reaction.

Higher the temperature means more  
energy acquired by molecules,  
which means a lower activation energy.

That means more collisions,  
which will further increase the  
rate of the reaction.

We have also seen the Arrhenius equation  
and we have seen the formula to  
calculate the activation energy  
at two different temperatures.

These are my references.

Thank you.