

**Concepts of Chemistry for Engineering**  
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**Lecture 62**

**Intermolecular forces: Dipole-dipole, hydrogen bonding and van der Waals interaction**

Hello everyone, welcome to the module on intermolecular forces, and potential energy surfaces. We are still discussing the interaction between molecules and what kind of form they are and what are the consequences of that. And in this particular lecture, we shall look at permanent dipole, permanent dipole interaction and hydrogen bonding and van der Waals interaction in a little more detail.

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**Brief recap**

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1. Why study intermolecular interactions
2. Different kinds of intermolecular interactions
3. Ionic and ion-dipole interactions



But before we jump into the permanent dipole, permanent dipole interaction, let us just quickly recap what we learned in the previous class. In the previous lecture, we first looked at why do we need intermolecular interactions or why should one even study intermolecular interactions and what is the role of it in chemistry, biology and material science.

Then, we looked in to the different classification of intermolecular interactions based on whether it is charged or whether it is polar and the different subclasses of that. And after that, we had looked at in a little more detail the ionic, as well as the ion dipole interaction. And we had looked at in specifically the one the distance dependence or of the potential energy of interaction between the two species which are interacting and we had said that the ionic interaction which goes as  $1/r$  is a long range interaction.

So, in this particular lecture, what we shall do is, we shall go a step ahead that is going from an ion dipole to a two-permanent dipoles and see how does the interaction potential of such a system look like?

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### 3. Permanent dipole – permanent dipole interaction

$$V(r) = \frac{q_1 q_2}{4\pi\epsilon_0 r} \quad \text{— General}$$

$$V(r) = \frac{q_1 q_2}{4\pi\epsilon_0 r} - \frac{q_1 q_2}{4\pi\epsilon_0 (r+l)} - \frac{q_1 q_2}{4\pi\epsilon_0 (r-l)} + \frac{q_1 q_2}{4\pi\epsilon_0 r}$$

$$V(r) = \frac{q_1 q_2}{4\pi\epsilon_0} \left\{ \frac{1}{r} - \frac{1}{(r+l)} - \frac{1}{(r-l)} + \frac{1}{r} \right\}$$

Let us start looking at a permanent dipole - permanent dipole interaction. So, what we shall do is we shall have a couple of assumptions, that is, the both the interacting dipoles are point dipoles and they are interacting in plane and along a collinear line in the plane of the board. This would make us easier to derive the expression first, and then, we can add on certain conditions to look at a more realistic picture.

Now, let us say we have a one-dipole moment which is I am showing it here the two charges that is let us say  $Q_1$  and minus  $Q_1$ , and they are separated by a distance  $l$ . And, now, I have another point dipole, which is separated by again a similar distance  $l$ . I will call this  $Q_2$  and minus  $Q_2$  and this again separated by distance  $l$ , and both of these are separated from each other by a distance  $r$ . And I am representing  $r$  from the midpoint of this interaction between the individual dipoles and this is  $r$ .

Now, what we will do is, we shall apply our same equation of potential between the interaction potential for two points or just that is  $V$  have  $r$  is equal to general formula  $Q_1, Q_2$  divided by  $4\pi\epsilon_0 r$ . So, this is the general equation. Now, what we will do is, we will take  $Q_1$  and look at the interaction of  $Q_1$  with  $Q_2$  as well as minus  $Q_2$ . Similarly, minus  $Q_1$  interacting with  $Q_2$  and minus  $Q_2$ .

So, now let us go ahead and look at how does that potential look like. So,  $V$  of  $r$  is equal to  $Q_1 Q_2$  divided by  $4\pi\epsilon_0 r^2$ . And if you now look at the distance between  $Q_1$  and  $Q_2$ , it is actually  $r$ , because you can displace the  $r$  from the center point to let us say the starting charge that is a  $Q_2$  and  $Q_1$  and you would see that, that distance is equal to  $r$ . So, this distance would be now  $r$ .

And now I am going to look at  $Q_1$  interacting with minus  $Q_2$ . So, the term would be minus  $Q_1, Q_2$  divided by, again,  $4\pi\epsilon_0 r^2$ . Now the distance would be slightly higher, because I am looking from  $Q_1$  to the minus  $Q_2$ . And if you now look at the distance by geometric arguments, you would see that this distance would be  $r + l$ . So, you can try and first look from  $Q_1$  to  $Q_2$ , that distance is  $r$  and from  $Q_2$  to minus  $Q_2$  is  $l$  so I am adding the distance  $l$  here.

So, then, I will add a, I will go and look at how does minus  $Q_1$  interact with  $Q_2$ , so that would again be a minus term  $Q_1, Q_2$ , divided by four  $4\pi\epsilon_0 r^2$ . And this time, you would see that this distance would be  $r - l$ . Because if I take a look at the distance between, say  $Q_1$  and minus  $Q_1$  and minus  $Q_2$ , that would be  $r$ . And to get distance between minus  $Q_1$  and plus  $Q_2$ , I need to subtract the distance  $l$ , which is the length of this dipole. So, that is why I have a minus term here.

And finally, I am looking at the interaction between minus  $Q_1$  and minus  $Q_2$ , and that would be positive  $Q_1, Q_2$  divided by  $4\pi\epsilon_0 r^2$  and the distance would be  $r$ , I hope that is easy to understand. Once we have got this potential form, then what we will do is, we will try and simplify this a bit further, and let us go ahead and see that.

Now,  $V$  of  $r$  potential is equal to, I can take out  $Q_1, Q_2$ , and  $4\pi\epsilon_0$  out then I would be left with  $1/r - l$  divided by  $r + l$  minus  $1/r - l$  divided by  $r - l$  plus  $1/r$  divided by  $r$ . I hope, this is clear to everyone. So, once we have done this, now let us go ahead and look at a little more simplification of this.

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### 3. Permanent dipole – permanent dipole interaction: continued...

$$\begin{aligned}
 V(r) &= -\frac{Q_1 Q_2}{4\pi\epsilon_0} \left\{ \frac{-2}{r} + \frac{1}{(r+a)} + \frac{1}{(r-b)} \right\} \quad \left[ \frac{Q}{r} \right] \frac{1}{(1+x)}, \frac{1}{(1-x)} \\
 &= -\frac{Q_1 Q_2}{4\pi\epsilon_0 r} \left\{ -2 + \frac{1}{\left(\frac{1+a}{r}\right)} + \frac{1}{\left(\frac{1-b}{r}\right)} \right\} \quad \frac{1}{(1+x)} = 1 - x + x^2 - x^3 + \dots \\
 &= -\frac{Q_1 Q_2}{24\pi\epsilon_0 r} \left( -\frac{2}{r} + \frac{1}{r} + \frac{1}{r} \right) \quad \frac{1}{(1-x)} = 1 + x + x^2 + \dots \\
 &= -\frac{Q_1 Q_2}{24\pi\epsilon_0 r} \left( -\frac{2}{r} + \frac{1}{r} + \frac{1}{r} \right) \quad \frac{1}{(1+x)} + \frac{1}{(1-x)} = 1 - x + x^2 - x^3 + \dots \\
 &= -\frac{Q_1 Q_2}{24\pi\epsilon_0 r} \left( -\frac{2}{r} + \frac{1}{r} + \frac{1}{r} \right) \quad + 1 + x + x^2 + x^3 + \dots \\
 &= -\frac{Q_1 Q_2}{24\pi\epsilon_0 r} \left( -\frac{2}{r} + \frac{1}{r} + \frac{1}{r} \right) \quad = 2 + 2x^2 \\
 &= -\frac{Q_1 Q_2}{24\pi\epsilon_0 r} \times \frac{r^2}{r^2} = -\frac{\mu_1 \mu_2}{24\pi\epsilon_0 r^3} = V(r)
 \end{aligned}$$

So, I am going to write the same expression here  $V$  of  $r$  is equal to  $Q_1, Q_2$  divided by  $4\pi$  epsilon naught. And so now, what I would do is, I would take a minus out and I would also take out  $r$  from that previous expression, then that would leave me with  $2$  plus  $1$  divided by  $r$  plus  $1$  plus  $1$  divided by  $r$  minus  $1$ , I think this will be minus  $2$ , yes. So, this would lead me to this particular term. And let me just not take out the  $r$  yet, so I would have  $2$  by  $r$ .

So, then the next step, what we will do is, I have just taken out a minus sign, so then I would get this particular expression. And in next step, I will take an  $r$  out from the denominator. So, minus  $Q_1, Q_2$  divided by  $4\pi$  epsilon naught, I taken the  $r$  out so this is minus  $2$  plus  $1$  divided by  $1$  plus  $1$  by  $r$  plus  $1$  divided by  $1$  minus  $1$  by  $r$ . So, we shall just now look at just these two terms, and see, if we can simplify them further.

So, I can write  $1$  by  $r$  is equal to  $x$ , so then this term would become. I am just looking at these two terms. I will come back and put it into this in a minute. So, it will become  $1$  divided by  $1$  plus  $x$  and the second term would be  $1$  divided by  $1$  minus  $x$ . And in order to understand or in order to expand this, solve for this, we shall make use of what are called as Taylor expansion. And the Taylor expansion series for  $1$  divided by  $1$  plus  $x$  is equal to  $1$  minus  $x$  plus  $x$  square minus  $x$  cube, and so on.

Similarly, for  $1$  divided by  $1$  minus  $x$  is equal to  $1$  plus  $x$  plus  $x$  square plus so on. If you apply these two to the terms here, which I have written on top, let us say these terms, then what I would get is,  $1$  divided by  $1$  plus  $x$  plus  $1$  divided by  $1$  minus  $x$  would be equal to  $1$  minus  $x$  plus  $x$  square minus  $x$  cube, so on plus  $1$  plus  $x$ , plus  $x$  square plus, plus  $x$  cube plus so on. So, I hope now you can see that I can, these two terms actually gets cancelled the  $x$

terms, and similarly the odd powers get cancelled, and all you are left with is the even powers. And we can neglect the higher terms because the  $l$  is smaller, much, much smaller compared to  $r$ , so this would actually reduce to  $2 + 2x^2$ ,  $2 + 2x^2$ . So, if I take this now, and come back, and put it here, then I would have the following.

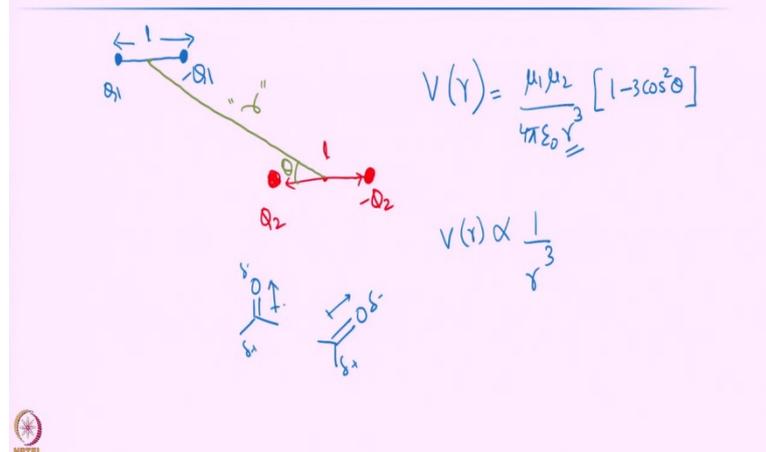
Minus  $Q_1, Q_2$  divided by  $4\pi\epsilon_0 r^2$ , plus  $2 + 2x^2$ . So, these two terms get cancelled, and here I will have left with  $2$ , and this will be equal to minus  $Q_1 Q_2$  divided by  $2\pi\epsilon_0 r^3$  times  $x^2$ . And I know that  $x$  is equal to this particular formula, that is  $l$  divided by  $r$ , so I am going to write as  $l^2$  by  $r^2$ . And we can do a very similar thing as we did for the ion dipole, that is, if I have the length  $l$ , multiplied by the charge  $Q_1$  or multiplied with the charge  $Q_2$ , then I would end up in the corresponding dipole moment vector, that is  $\mu_1$  or  $\mu_2$ .

So, if I take help of that equation, then this would reduce to minus  $\mu_1, \mu_2$  divided by  $2\pi\epsilon_0 r^3$ . So, this is I am just going to write it here as  $V$  of  $r$  and this is the key equation, which ultimately governs the dipole-dipole interaction. And the negative sign indicates that there is an attractive force between the two species. And the most important or the striking thing to notice that it goes as  $1/r^3$ , that is, as the third power of the distance between the two dipoles or the center of the distance between the two interacting dipoles.

So, this is a very important thing to keep in mind. And as I said previously, this was all for simple two dipoles actually interacting in a collinear manner on the plane of the paper, but that is a bit of an idealized situation. So now let us see what happens if the two dipoles are at an angle.

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### 3. Permanent dipole – permanent dipole interaction: *Angular dependence*



Now, let us look at the angular dependence of it. And in order to do that, I will again go back and draw the dipole moment picture, that is, I have one dipole here  $Q_1$  minus  $Q_1$  with a distance  $l$ , and the other dipole I am going to draw somewhere not collinear with it. This is  $Q_2$  and minus  $Q_2$ . So, I hope, you now see that there is actually the angular term or the angle between these two dipoles or the center of these two dipoles also becomes an important factor now. Not just the distance between them. So, I shall try and draw the distance between these two that is.

So, this is the  $r$  that is the distance between the two dipoles and now this  $\theta$  or the angle which is the two dipoles are making with respect to one another is also an important factor or component to take when we want to look at the potential of interaction between these two systems.

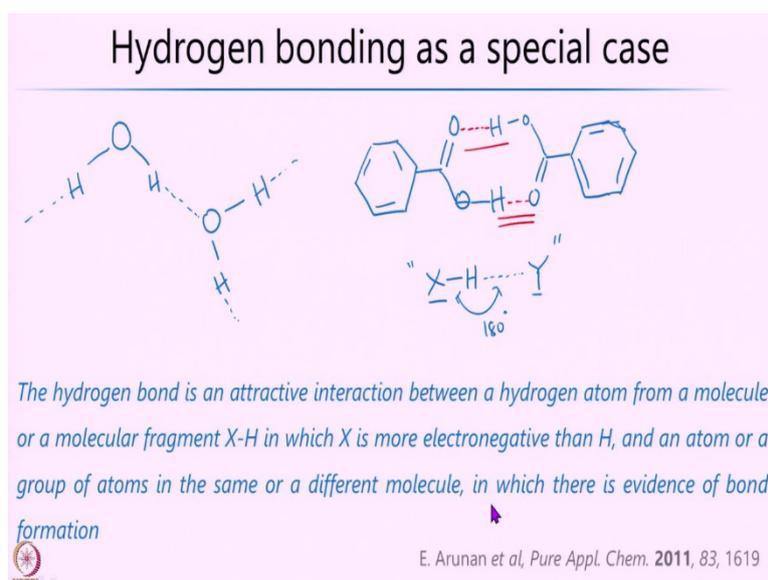
If we take that into account then the potential would look like the following that is  $V$  of  $r$  is equal to  $\mu_1, \mu_2$  divided by  $4\pi\epsilon_0 r^3$  the distance dependence does not change the  $r^3$  remains, however, you will have a new term that is  $1 - 3\cos^2\theta$ , this is an important part to take into account the angular dependence between the two dipole moments which are now actually within the same plane, but at a different angle, acting at different angles with respect to each other.

However, you can also think that this is one possible condition or one possible scenario. What could also happen is that I can have two dipole moments actually may not be in the same plane, they could actually be in two different planes like this, one is in this plane another is in this particular plane.

So, in this case you will have one more angular part which will actually come into picture and that would slightly make the equation for  $V$  of  $r$  a little more complex, but what would remain same is the distance dependence, which is this, the  $1$  by  $r$  to the power  $3$  are  $V$  of  $r$  the proportionality of  $1$  by  $r$  to the power  $3$  would remain constant and that is something which is very significant and which we need to keep in mind.

So, having talked about dipole moment a permanent dipole, permanent dipole let me just give you an example of this to see what kind of systems one looks at. Say, if I have a molecule of an acetone, which is interacting so, this is one particular example where I have two dipoles which are now interacting at a certain angle, and this equation can be used to calculate the dipolar interaction between these two molecules which are actually non-charged or uncharged, but they are still polar or they have a permanent dipole moment. Now, let us go ahead and try to look at a hydrogen bonding as a special case of the dipole-dipole interaction or permanent dipole permanent dipole interaction.

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So, I am sure, when I say hydrogen bonding you will start thinking about water or the system which we talked about earlier that I had shown you that we had oxygen, which was bonded to two hydrogens. And what I can also do is, I can write another oxygen and I can write two more hydrogens here like this. And you can draw this interaction as a hydrogen bond and so on and so forth. You can keep on writing like this as a chain of hydrogen bonds.

This is what would keep the water molecules interact with one another in a glass of water. And there are different forms of hydrogen bonding as well. That is, you can also write for let us say for example, if you take benzoic acid. So, here again, what you see is that there is a

interaction between the two systems that is this is the interaction, which is the interaction between a hydrogen which is attached on the OH and a carbonyl oxygen, similarly on top.

So, people typically observed that if X-H system, which is interacting with the Y then, and if given that X and Y are two electronegative atoms which are more electronegative than hydrogen, then typically you would have what is called as a hydrogen bonding interaction. And this the strength of the interaction would depend heavily on, one, the difference in electronegativity between X and Y and also the angle at which the X-H and Y is coming in.

If they are coming in like at 180 degrees that is this angle, then you would have the maximum interaction possible. However, if they are coming in at a slightly different angle, then the interaction strength would actually decrease. So, this is a classic example of hydrogen bond in a system such as water or a benzoic acid. And people have actually argued and debated about the hydrogen bonding extensively in the literature.

And what has come out from this is the following definition. That a system is said to, a hydrogen bonding is said to be there in a system, if there is an attractive interaction between a hydrogen atom from a molecule or a molecular fragment X-H in which X is more electronegative than hydrogen and an atom or a group of atoms in a same or a different molecule and in which there is an evidence of bond formation.

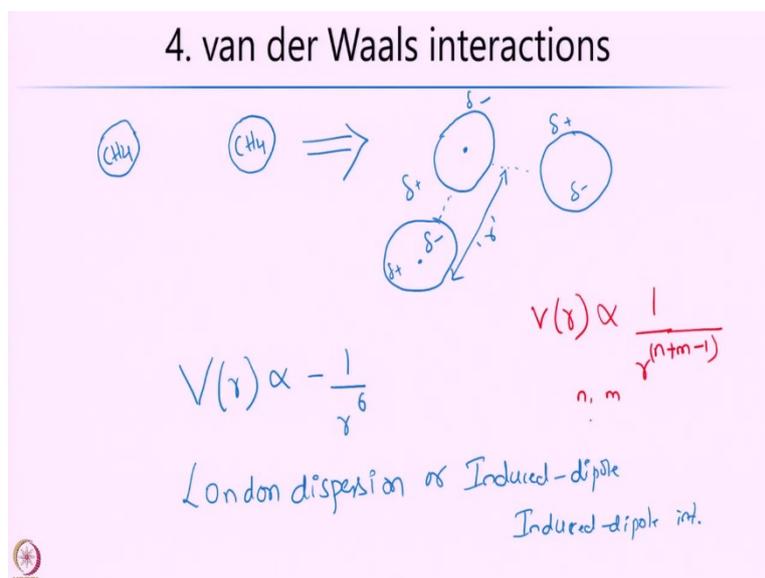
So, this is a very sort of recent and accepted definition of hydrogen bond, which is come about by a group of scientists from all over the world sitting together and debating and coming up with this this definition. So, all this tries to do is, to capture many different flavors or many different forms of hydrogen bonding. And the basic essence is that the hydrogen should be planked between two electronegative atoms that is X and Y and there should be an evidence of bonding.

So, at this point, you might be thinking so, how can I classify hydrogen bond? Should I call it as electrostatic? Should I call it as a permanent dipole, permanent dipole or how do I classify it? So, that is the reason, why we have called it as a special case because in the literature or in the scientific research some people attribute it as a electrostatic in origin or it has primarily electrostatic origins, and some people call it as a dipole-dipole origin.

So, that is actually not very clear to or easy to separate. Both factors actually too play a role that is, electrostatic interaction as well as the dipole-dipole interaction do play a role in giving rise to a hydrogen bond. So, with this in mind, we shall just call it as a special case and the

strength of this interaction would depend heavily on what are the two different atoms X and Y and also what is the angle at which these two species are interacting with one another.

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So, now, we shall actually move on to the last class of interaction which are typically called as Van der Waals interaction or also called as London Dispersion or induced dipole, induced dipole interaction. Let us go ahead and try and see for which kind of systems this interaction plays a role.

So, previously, we had seen that, if we take a molecule like say CH<sub>4</sub> non-polar. So, if you take a non-polar and also non-charged system like methane, ethane, argon or different kinds of inert systems, so then, there would not be any apparent interaction one could think of. However, if you go back and look at your lectures on quantum mechanics, what you will realize is that the electrons in a system in a molecule or in a particular bond is actually never stationary, it is always oscillating around the, in a given space, where the probability of finding the electron is maximum.

So, this moment of electron or the continuous, let us say the oscillation of electron would give rise to what are called as induced dipoles or induced charges in a system. So, if I take this particular system and this would probably give rise to something like say, a delta plus and a delta minus in the same molecule itself, and this is just instantaneous. It is not something, which is which you can find if you take a molecule of methane or an ethane, it is just instantaneous, which is formed on a timescale as the electron redistribution takes place.

So, once this happens, you will also have another neutral molecule which is actually floating around. And if this comes in close contact with this, what can happen is, that this can start inducing the charge that this will give you a delta positive here, and this part if it comes in close contact, this would induce a delta negative and a delta positive here.

So, now, what you have is, the electron redistribution in a molecule is actually now giving rise to induce dipoles like what I have shown here by the partial charges, and these induced dipoles actually interact with one another in a molecule. And this is what one calls it as a van der Waals interaction or also called as a London Dispersion forces or also called an induced dipole induced dipole interaction.

And the form of the potential is the following that is  $V$  of  $r$  is I will just write the distance dependence that is  $1$  minus  $1$  by  $r$  to the power  $6$  that is it goes as the  $6$ th power of the distance between the two interacting molecules. For example, if I take here this is the center and this is the center then this would be the  $r$  and the interaction potential would decrease very, very rapidly.

So, I guess, you can see that the van der Waals interactions are actually very close contact interactions or they would only come about or become significant when two molecules are nearby or close to each other. And the moment they actually go a bit apart, the interaction falls off very quickly. So, this is what people would typically also call as London Dispersion or induced dipole, induced dipole interaction.

So, so far, we saw many different kinds of interactions ranging from interaction between two-charged species to interaction between a charged species and a dipolar system to two dipoles system to two completely non-charged and non-polar system, such as a methane, ethane or any such inert systems.

So, if I were to write a general formula to get the interaction potential as a function of  $r$ , then that potential would be of the following form. So,  $V$  of  $r$  would be  $1$  by  $r$  to power  $n$  plus  $m$  minus  $1$ . So here,  $n$  and  $m$ , are the, let us say the  $n$  and  $m$  correspond to the poles which are interesting. That is if I have a dipole, which is interacting, that means there are two charges interacting, so  $n$  becomes  $2$ .

And then let us say I am having an dipole interacting with a charged species, so then the  $m$  is  $1$ , so then  $2$  plus  $1$ , that is  $3$  minus  $1$ , then that would give me an  $r$  square, which is exactly what we saw for an interaction between a point dipole and a dipole, between a point dipole

and a charged species, So,  $n$  and  $m$  corresponds to the dipolar state of the two interacting species. So, having looked at various systems, now let us go ahead and try to summarize what we have learned in this lecture about intermolecular interactions.

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Type of interaction	Interaction energy	$V(r)$
Ionic	200 – 400 kJ/mol	$1/r$
Ion – dipole	10 – 80 kJ/mol	$1/r^2$
Dipole – dipole	5 – 30 kJ/mol	$1/r^3$
van der Waals	< 5 kJ/mol	$1/r^6$

So, I have shown you this particular diagram where there is a spectrum of interactions going from a completely charged species the interaction between two charged species to a completely to a interaction between two completely nonpolar, and uncharged species.

So, if you were to look at the interaction strength and the distance dependence of the potential, then at the top, we have the ionic interaction, which we also call it as a long-range interaction, that is interaction between two ions, and this is in the range of about 200 to 400 kilojoules per mole, and it goes as  $1$  by  $r$ .

And next, what one can have is I can replace one of the ions by a dipole, then I will have an ion dipole interaction. And this would actually now have a significantly lower interaction strength, because I no longer have two-charged species. I am looking at one charged and one uncharged species. And this would be somewhere around 10 to about 80 kilojoules, depending on the specific system we are interested in and that would give a  $1$  by  $r$  square dependence of the potential.

And if we go ahead further and replace the first ion by another permanent dipole, then I get a permanent dipole, permanent dipole interaction. And this interaction strength would be somewhere between 5 to about 30 kilojoules per mole, again depends on the particular

system we are looking at. And the interaction potential would go as  $1/r^3$ , which we looked at by looking at the derivation.

And finally, in the last slide, we saw that if we now replace both the polar molecules by completely a-polar molecules such as methane, ethane or argon, then one would end up in water called as London Dispersion or van der Waals or induced dipole induced dipole interactions. And this interaction strengths are very, very small that is out the order of 5 or 5 to 10 kilojoules per mole at the max. and these are very short-range interactions, meaning, they actually fall off as the 6th power of the distance between the two interacting systems.

So, what this tells us is that the induced dipole induced dipole interactions or van der Waals interactions are very, very short range very, very short-range interactions. And the moment you actually go to a larger separation they actually fall off, whereas, the ionic interaction and ion dipole or to an extent dipole-dipole interactions are long-range meaning they can interact with systems which are much farther away from the parent system.

So, with this, we shall stop our discussion on intermolecular interactions. And in the next lecture, we shall look at what are the consequences of these intermolecular interactions on the properties of the gases that is real gases and also critical phenomena. Thank you.