Fundamentals Of Combustion (Part 1)
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Lecture – 12
Heat of reaction and bond energy

So, let us start this lecture with a thought process.

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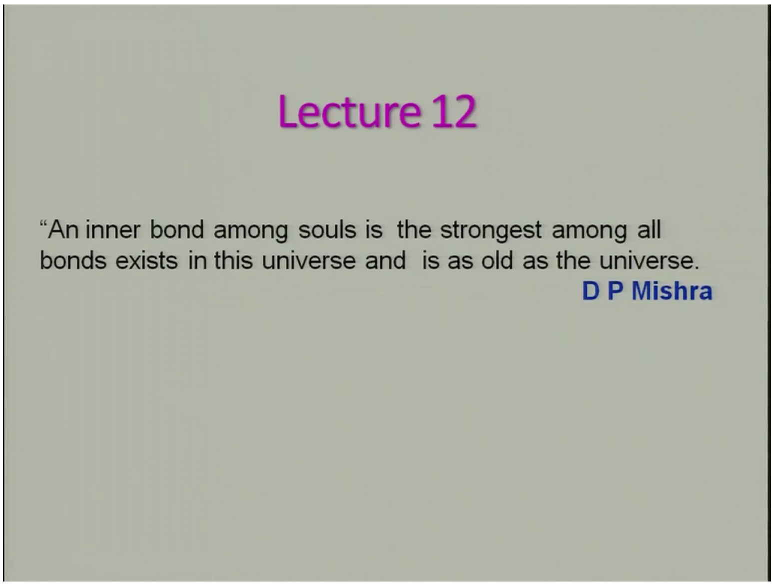

"An inner bond among souls is the strongest among all bonds exist in this universe and is as old as our universe."

If you look at like in the last lecture, we basically discuss about heat of formation and heat of reaction and heat of combustion. Then we learned how to calculate the heat of reaction from the heat of formation and then, knowing the heat of reaction, we also calculated the heat of combustion and keep in mind that we are using heat of combustion and the calorific value interchangeably and we also learnt how to estimate the lower heating values and lower calorific values or lower heating values or higher calorific values.

And if we look at like we basically determine the heat of reaction from heat of formation. That means, those things will be available in the table. Now suppose, there is a situation where those tables or the data's of the heat of formation a tabular form or any other is not available. Let us say you are developing a new compound, where you know the, you do not have data. So, how we are going to do that is the question.

So, for that what we will use? We will basically use the bond energy and then, calculate the heat of reactions. So, a question might be coming to your mind, what is bond energy? Of course, you know very well because bond energy was taught to you in plus 2 very extensively. I will be not discussing about that.

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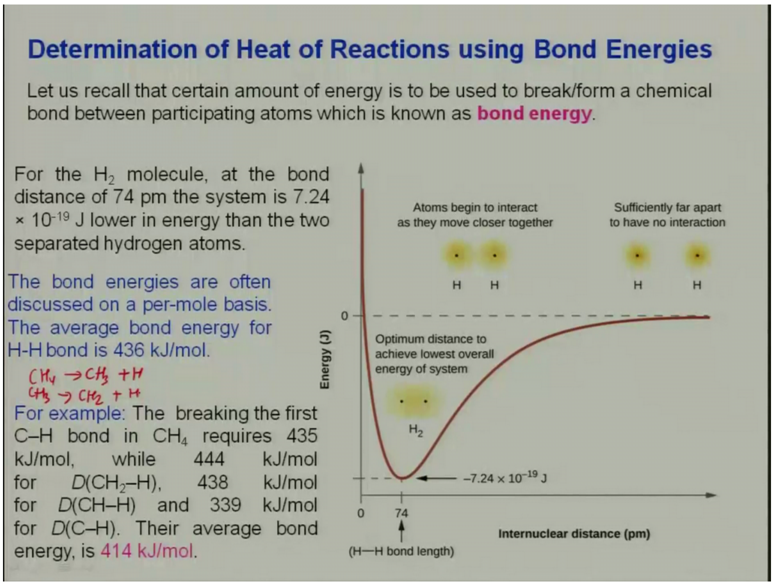

But I will just try to make you to recall that bond energy is basically the certain amount of energy that is being used to break or form a chemical bond. And we know that the chemical reaction means the breaking of bond or forming a new bonds; breaking up old bonds as are breaking a bonds as the forming of new bonds.

So, therefore, that is the energy, amount of energy which is required basically to have a bond between the you know elements and you might be knowing like just now, you know yesterday we had Independence Day. We are having lot of energy lot of money. We spend for celebration of Independence Day. What for? That is basically to reinforce the bond between the individual and the country. What is known as Patriotism am I right. So, to have because nowadays; internationalization is there.

Therefore, you know lot of this thing beside this also you should have some kind of obligation for your nation. So, that is also a vertical patriotic is one form of bond. So, you are having also what you call bond with your family; yes or no? Of course, there are various forms of bonds are there in a chemical reaction; covalent bond, ionic bond, hydrogen bond, you know like kind of things.

So, but how does it really form and why energy is required? Let us imagine that there are 2 H atom and when you talk about the atom; there will be nuclear, there will be electrons and these are very far apart.

That means, they are not interacting with each other. They will be very far apart and of course, the bond is strengthened wherever there will be interaction like for example, in ancient time the people were far apart.

There is no interaction. For example, when I went to my engineering college, you know I do not have an interaction with my parents except writing a letter, but today you are having more interactions; that means, more bond; is it so? Do you have better bond?.

Then, what it was previously? Of course, that is a debatable thing, we will not discuss now. Coming back to this that will be heaving you know 0 energy; we are considering that there is no interaction. Therefore, it will be having 0 energy here.

And as this you know atom will be coming closer; what will be happening? That means, there will be interaction between the nucleus and the electron of other hydrogen atom and also that there will be interaction with a nucleus to nucleus.

So, therefore, there will be you know when they are coming there will be 2 forces which will be acting. What are those 2 forces? One is the attraction or the cohesion you call; other is repulsive forces. In this case as they will be closer to each other; then, attractive forces will be stronger, repulsive forces will be weaker.

And till, what will happen? It will be coming to a minimum label, which is happens to be for this that is hydrogen molecule will be formed because that is the lowest overall energy of the system and the distance of course, the optimum and that distance is known as Bond length.

In this case it happens to be 74 Pico meter and the energy whatever is there is 7.24 into 10 power 2 minus 19 joule is a too small energy; is not it? It is a too small energy.

So, if it is there; then, what will happen? Like that will be the strongest bond will be formed like bond will be formed; in that case you know like you can say that the separation distance is the optimum one and this amount of energy is formed. But you know what we will do with this?.

This is too small energy, but when you talk about this bond energy is basically will be in terms of mole; whenever we will talking, we will be talk in terms of moles and you might be knowing according to the Avogadro's you know number. What is the Avogadro's number? Is basically at 6.23 into 10 power 23 molecules per mole at standard temperature and pressure; but, what will be the volume? Volume will be 22.7 litres.

So, what I am saying then, but we will be more interested not that a single hydrogen molecule is being formed by the, from the 2 this thing or any other thing, but rather we will be talking about in terms of moles.

So, the bondage is often discussed on a per mole basis. So, average bond energy for H H bond will be 436 kilo joule per mole. It is a quite a you know large amount of energy per mole; keep in mind that this bond energy is you know will be different than the dissociation bond energy.

What will be interested more interested in the average bond energy? I will take a example of methane. So, let us say the methane you know CH4 and CH4 from that you know 1 H atom is being extracted as a result there will be CH3 and H. CH4 will be let us say getting into CH3 plus H.

Then, what will be the, because 1 hydrogen, you know bond is being dissociated. So, what will be amount of energy that is required is something 435 kilo joules per mole. But if we will go for the next one that is CH3 will be converted into CH2 plus H. Then what will happen? That will be 438 kilo joule per mole. And again, similarly if it is CH2, CH plus H; then it will be something 438 kilo joules per mole.

And in the last one of course, that will be C and H that will be 339 kilo joule per mole, but if you take average of that you know because all our CH bond, if you take average, what you will get? You will get something 414 kilo joule per mole and that we will be using. But individually they dissociation, that will be different. So, you should keep that difference in your mind.

And of course, the tables should be available in the bond energy of various kinds of bonds and those are being estimated and tabulated and we can use that if you look at.

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Representative Average Bond Energies and Lengths

Bond	Length (pm)	Energy (kJ/mol)	Bond	Length (pm)	Energy (kJ/mol)
H–H	74	436	C–O	140.1	358
H–C	106.8	414	C=O	119.7	745*
H–N	101.5	391	C≡O	113.7	1072
H–O	97.5	464	H–Cl	127.5	431
C–C	150.6	347	H–Br	141.4	366
C=C	133.5	614	H–I	160.9	298
C≡C	120.8	839	O–O	148	146
C–N	142.1	305	O=O	120.8	498
C=N;C=N	130.0	615	F–F	141.2	159
C≡N;C≡N	116.1	891	Cl–Cl	198.8	243

* For CO_2; use 799 kJ/mol

This is given these are the H-H bond. Of course, there will be single bond, there will be double bond and you know some triple bond are there also, various thing. And these are bond length in Pico meter is given and these are energy which is given like H-H 436 SC or CH you know. SC or CH, whatever you call 414 like that it goes and similarly C-O and the other various bonds are given, keep in mind that when you use this CO2 and that will be you will have to when it is a CO2; basically C-O bond, the CO2, you will have to use 799 kilo joule per mole that is being you know given.

So, what will do? We can use this kind of data of the bond energies and estimate heat of reaction instead of using the heat of formation. Where we will be using that? Basically when those heats of formations are not available; well suppose you have developed a new company; where you do not have enough data or you cannot really measure the you know calorific values, let us say.

That compound you cannot use in a bomb calorimeter or a young cut calorimeter, you know and then find out. So, naturally you will have to use this kind of thing to check how much you know heat of reactions or heat of combustion is there or calorific value of any fuel.

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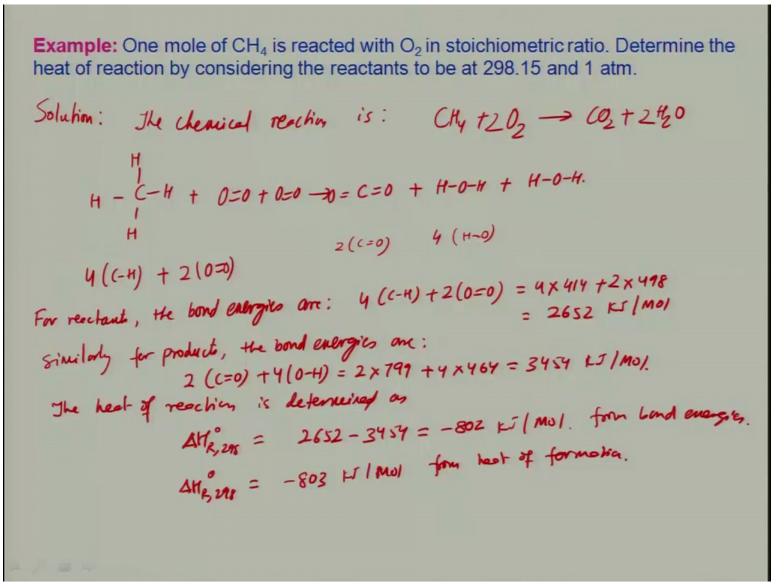

So, let us look at one mole of methane is reacting with the oxygen in stoichiometric ratio. Determine the heat of reaction by considering the reactants to be at 298.15 and 1 atmosphere pressure. The standard heat of reaction, what will be finding out and we will be using basically bond energy instead of heat of formation.

So, we know the chemical reaction will be CH 4 plus this is oxygen. So, this will be CO 2 plus water and this will be basically to balance it; this will be 2. That means, 1 mole of methane is react to meet 2 moles of oxygen, going to the product of 1 mole of carbon dioxide and 2 moles of water.

And now, if you look at what is C-H, C basically CH 4, CH 4 H, you know H plus there are 2 O 2. So, O plus double bond, and going to carbon monoxide, O plus H-O-H plus H-O-H. In this case, if you look at on the left hand side that is a reactant side, how many C-H bonds are there?.

This basically 4 bond. So, I can write down C-H 1 4 plus how many o bond is there? 2 O bond and the reactant side and going to the product is basically, how many bonds are there here. In this case there are 2 basically 2 C-O bond and this is 2 O-H-O bond; no 2 or 4? It will be 4 basically; this will be 4.

So, now let us calculate For reactants, the bond energies are: what it would be? It would be basically 4 C-H plus 2 O. So, if you look at the table, let me go back to the table. The H, will be what? C-H will be?

Student: 14.

14 and O-O. What is O-O?

Student: (Refer Time: 15:20).

Is?

Student: 498.

498 and then, in the product what will be? Will be using CO 2. So, we will be using this one, 799 and will be using O-H. O-H is basically 4.

Student: 464.

464. So, these data we are going to put into those things use them and then, find out what will be this thing. In this case what will be it 4 into 414 plus 2 into 498, it happens to be 2652 Kilo Joule per Mole. Similarly, for the product, the bond energy 2 plus 4 O-H 2 into 799 plus 4 into 464; it happens to be 3454 Kilo Joule per Mole.

Now, the heat of reaction is determined as delta H R. This is basically 298 and 0 and this is nothing but basically a reactant minus the product that is 2652 minus 3454 is happens to be something 802 Kilo Joule per Mole. Keep in mind that if you look at earlier example, when we calculated heat of combustion; what does the value, can you look at your note? Heat of reaction.

Student: (Refer Time: 17:54) minus 8 (Refer Time: 17:58).

Yes; that means, I got something minus 803.

Student: point (Refer Time: 18:03).

Kilo joule per Mole and that is from heat of?

Student: (Refer Time: 18:10).

Formation; Heat of formation. From that data, I got this delta H R basically heat of reaction; we are calculating from heat of formation. This is from bond energy. So, therefore, it is very close, but keep in mind that it need not to be very close to you know each other, but there might be some difference, but that difference may be small. Here it is too small; negligibly small, but in some cases it may be 5 percent, 6 percent difference will be there.

That means, you can really calculate both the ways heat of reaction and the heat of combustion either from by using the heat of formation data or using the bond energy data. So, this is the thing what I was you know trying to tell you and these things you most of you know, but only I am making you to recall and then reuse is. So, that you can use them in future, whenever it is required and this is basically being used when you do not have heat of formation data, you know; then, only you will use or when it is not possible to find out experimentally.

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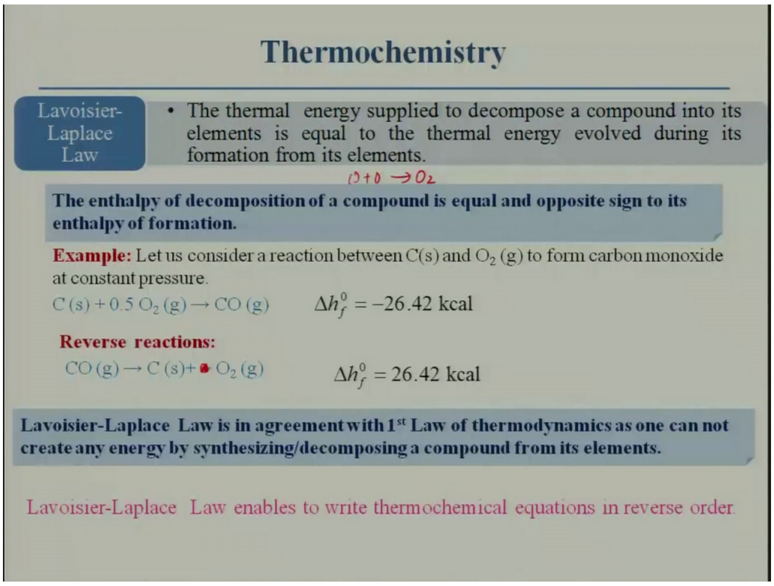

So, now to deal with you know this kind of chemical reactions and then associated heat liberation or heat being you know used in the chemical reactions depending on whether it is exothermic reaction or an endothermic reaction. We need to use certain laws; there are 2 laws which we will be discussing one is Lavoisier-Laplace law which says that thermal energy supplied to decompose a compound into its element is equal to the thermal energy evolved during its formation from its elements. What it indicates? Is it related to any law whatever you are aware?

Student: (Refer Time: 20:12).

It is basically?

Student: Conservation.

Conservation of energy; that is nothing but your First law of thermodynamics.

So, but this will be applied for the chemical reaction and in other words, what he says? The enthalpy of decomposition of a compound is same, but with a equal sign that of the heat of formation whenever you are having the decomposition.

For example, O. O and O is you know reacting going to the O 2; that means, this is basically heat of formation and on the backside, it will be also same thing. That is the point, what he is saying opposite sign. For example, let us say that carbon is reacting with oxygen to form carbon monoxide at a constant pressure.

Then, what we need to do? I mean we will have to basically, you know it is balanced you can say you know like 1 mole of carbon is reacting with half moles of oxygen, going to the carbon monoxide. Of course, keep in mind that carbon is in solid phase and the oxygen and carbon monoxide is in gas phase.

And for this, the heat of formation is 26.42 kilocalories. Of course, you must be knowing that calories and the joule. One kilo calories is equal to 4.18 kilo joule. Basically, 1 kilo calorie is equal to 4.18 kilo joule. So, if you look at the reverse reaction that is carbon monoxide is converted into carbon and oxygen.

Then, it will be same, but delta H f is equal to 26.42 kilocalories. But keep in mind that this is basically with a positive sign that is all and. So, as I told that Lavoisier-Laplace law is in agreement with the 1st law of thermodynamics as it is not possible for any chemical reaction to create some energy or maybe destroy it. It can only convert 1 form to the another.

So, that is the basically it talks about the 1st law of thermodynamics and this will be in case of basically an isolated system. Can it be applied for the other system? When there is a heat interaction; then, it is actually heat will be convened into work or work will be converted into heat, but here there is no work, there is no heat being transferred. So, therefore, you are considering as a basically isolated system.

So, and that is nothing, but your 1st law of thermodynamics. So, how we use it we let me know, but I am just trying to summarize it Lavoisier-Laplace law enables us to write the thermo chemical equation in reverse order; the forward direction or the reverse direction heat of reaction will be same.

So, will this stop over here. In the next lecture will be discussing about another thermo chemistry law and that is known as chase law. So, we will discuss that in the next lecture.

Thank you very much.