Introduction to Explosions and Explosion Safety Prof. K. Ramamurthi Department of Mechanical Engineering Indian Institute of Technology, Madras

# Lecture - 13 Energy Release in a Chemical Reaction: Moles, Internal chemical Energy, Standard Heats of formation

Good morning, in today's class we will address the issue of energy release. You know whenever we have been talking of explosions what did we say.

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At some point or at some source some energy e naught gets released and what we ultimately get is, if the energy release is spontaneous we get a blast which does the damage. Therefore, the essence of an explosion is, that the energy should be released and that too it must be released fast enough. Therefore, today we will take a look at how to determine energy release and we consider one specific example or one specific case. We look at the energy release in the case of some substances, which can undergo chemical reaction.

You know such substances which undergo chemical reactions are also known as explosives. Let us first be very clear what we means by an explosive and for that we will take a few examples. Let us consider a substance let us say like hydrogen, hydrogen gas. Let us say I consider hydrogen gas and it is available in the market in cylinders. These cylinders are filled, here you have a regulator. The cylinder is filled with hydrogen gas and whenever we want hydrogen gas we tap it from the cylinder.

Well the hydrogen gas we say is little dangerous handle it carefully, but if I were to take this hydrogen gas in to this, if I take this example of hydrogen gas. I put an electrical spark in it or I heat it and nothing is going to happen. The hydrogen gas is not going to react and generate a large volume and generate an explosion because it is just a fuel, it is just a fuel by itself can not react and form products of combustion.

These products cannot really go to high temperature, even if I eat it only the sensible heat of hydrogen is going to increase. May be a similar example I can say well I go to the market and buy kerosene may be I buy kerosene in a pale let us say. If I isolate this kerosene oil let us say kerosene oil. If isolated from the air and heat the oil nothing is going to happen only may be it will vaporize, but unless it mixes with air and then reacts with air then only some combustion or an explosion can take place. Therefore, we say when a fuel or a substance like fuel like hydrogen may be methane, ethane any substance you take are not really substances which are explosive.



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Therefore, we talk in terms of fuels and these fuels could be either a gas. Like we talked in terms of hydrogen gas we could have may be methane, ethane could be a liquid, could be a volatile liquid like petrol, may be kerosene. It could also you have solid like you have wood, but wood contains little bit of oxygen we will take a look at it. May be these are the substances. Let us take an example, we talked of the largest man made explosion.

We said this happen in the Eural mountains in Siberia around June 4 th, I think it was 1979 or so. What really happened in this case, you know you had the pipe line which was conveying natural gas. Natural gas in nothing but methane a huge spill take place that means the rupture in the pipe line over a long distance happened. Lot of this methane got spilled over gaseous methane and we have low temperature methane gas.

What happened, along the ground the methane gas just kept on traversing, nothing really happened in this particular explosion because initially because methane just kept hugging the ground and kept on travelling because the wind took it across. What really caused the explosion may be we said there you had the trans-Siberian railway that means you have double track railways trains going in opposite directions. Then, it so happened unfortunately the two trains were passing through this cloud of methane gas at the same time in opposite directions.

When these two trains where passing in the opposite directions, they introduced turbulence they introduced mixing with air and along with mixing of air, you had an ignition source like you had the spark from the overhead cable and that caused a giant explosion. We said this particular explosion decimated the vegetation around this particular place of the explosion. Therefore, we say well in this case you had methane and methane is just a fuel it cannot itself. I need air to be able to form a combustible substance.

Therefore, we define an explosive as a substance which contains fuel and an oxidizer with which it can react and form products of combustion, which are at high temperature and probably at high pressure with which an explosion can get started. Therefore, let us now take a view on this well. It need not be only a gaseous fuel like methane and air.

It could be any substance therefore, let us take a look at different types of explosives. We talked in terms of Texas City disaster. Well this happened around April 1947or so. What happened in this case, you had ammonium nitrate. What was the formula for ammonium nitrate NH 4 no 3. The ammonium nitrate was stored in bags in the hall of a ship and it started reacted spontaneously.

How can something a substance start reacting. You know it started reacting slowly and all of a sudden the reaction built up. Therefore, if you look at a substance like ammonium nitrate it is not a mixture. It is not a mixture like methane and air or you have hydrogen mixing with air to form a combustible. It is a compound, it is a homogeneous compound and what is happening if you look at this particular compound, if I take a look at it well I have 2 nitrogen molecules, 2 nitrogen atoms. I have 4 hydrogen atoms and I have 3 oxygen atoms.

Therefore, it is quite possible, may be the nitrogen atoms of let us consider for the present day scene at and the 4 hydrogen atoms can react with 2 oxygen atoms to form 2 h 2 o, that means 2 water molecules and we are left with one oxygen atom. Therefore, it is quite possible that the hydrogen in the ammonium nitrate can react with oxygen in the same ammonium nitrate and form a chemical reaction which can generate energy.

Therefore, we say the ammonium nitrate could be an explosive. Therefore, explosives are those substances which contain fuel and oxygen within this particular substance, it could be a mixture of 2 things may be, I just mix some solid oxidizer with solid fuel. I mix it, that is it is heterogeneous it could again be an explosive or it could be a chemical compound in which fuel and oxygen fuel and oxidizer are intimately mixed. Therefore, whenever we talk of an explosive we mean, well I have fuel and oxidizer which are present. If I consider only a fuel well the fuel has to get out find air like in the explosion at Eural mountains, where in may be methane had to get mixed with air to form an explosive. That means initially I just had fuel and then I formed this mixture which if ignited forms the products of combustion.

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We are interested in finding out what is the energy released in the particular explosion. Let us take one more example to make sure we are on the right track. I take the example of the accident at flixborough. You know I was particular to take this example because many of you would go and work in chemical plants in the future or in some plants which handles chemicals. What happened in this particular plant. You know there was a major disaster, I think it was around June 1 1974, what happened in this case. You know the flixborough plant this is in UK, was making some intermediate known as caprolactum.

This intermediate or a precursor is used in making nylon. You know how you make this precursor caprolactum. You know you have in a chemical plant, you know you have these reactors there where something like 1, there were 6 reactors one after the other. Let us say you have 6 reactors and what happens may be what they used is cyclohexane. May be we are talking of hexane c 6 h 14, in the cyclo mode, that means it is not normal hectane, but it is in a cyclical chain.

What is done is this particular hexane or we say well it gets oxidize and you keep on oxidizing it in the different reactors until you found say caprolactum, which is used for making nylon. Therefore, you have these different reactors and what is done is form one reactor, the substance goes to the next. It gets oxidized, again it goes to the next, it goes to the next it goes to the next and this is how and ultimately you get whatever you want.

In this particular case there is particular cyclo hexane was being converted to hexonol hexonone and stuff like that.

Let us not get into too much of these details, but what happened is a few days before this explosion, you know you have something like 6 reactors. The reactor number 4 developed a small crack and therefore, what was done is, see now you have a number reactors you can always do without one. Therefore, what was done was one of this rectors was shut off and the product from this rector was connected through a bypass line to the next reactor, that is from third reactor it goes to the fifth reactor. This by pass line was something between 0.1 to 0.2 meter in diameter.

Well, you know during operation this particular bypass line developed a crack and the hexane or the cyclo hexane or hexonol which leaked into it, something like what the leak was so rapid that something, like forty tons of cyclo hexane leaked out. This was because the reactors are essentially operating at pressure. In this case it was operating at a pressure of 10 atmospheres and the temperature here was something like 145 degrees centigrade. Therefore, what happened is forty tons of cyclo hexane leaked out.

You form a huge cloud, a cloud of cyclo hexane mixes with air. You found a mixture of hexane and air and the size of this cloud was something like between 100 meters to 200 meters diameter that means it is a huge cloud of this vapor mixture which is formed which is now, an explosive because you talk in terms of hexane c 6 h 6, it is mixing with air and air contains oxygen, air contains nitrogen, we will take a look at the proportions a little later.

Therefore, in presence of the vapor of cyclo hexane that is hexane and oxygen it can react and you form this cloud of the explosive. When it formed you know in a chemical plant you have furnaces and other things which are always hot it finds an ignition source may be in a furnace in some hot spot. The whole thing just releases the energy and the magnitude of energy release was so high, it was something like 60 into 10 to the power 2 Jules of energy got released.

You know this is what we are interested, we want to find out when I have an explosive a given quantity of explosive, how much energy is getting released. What is it we have done so far, we know once I know how much energy is released and this is what we have done. We say well e naught I know, therefore I can calculate my explosion length being

e naught by p naught to the power 1 by 3. In this case with 60 into 10 to the power 12 and p naught being 10 to the power 5 Pascal, the value is something like almost like 80, it will it will come up to a few 100 meters something like 180 meters or so.

If I am interested in the over pressure, due to this explosion taking place and it was told that this explosion was so strong that this town ship of flixborough at a radius of something like almost 2 meters, 2 kilometers around the site of explosion was devastated. Buildings got totally damaged and therefore, using this value of r naught and may be at a distance of 2 kilometers that is 2000 meters I can find out the value of r s by r naught.

Then determine the value of over pressure which we now know how to do, we know how to calculate the impulse and we also know how to calculate the fragments which are thrown out. Therefore, what is primarily is the energy release from such explosions and this is what we do today. Therefore, let us comeback to our problem. Therefore, we say well in any explosion, the first thing required is how much energy is released in an explosion.

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Let us try to find that out, how much energy is released. You know we are talking of energy released in a chemical reaction and therefore, we tell ourselves whenever we talk of chemical reactions, what is the chemical reaction we are talking of in the flixborough. We say well c 6 h 14 hexane plus may be air forms may be products of combustion, could be carbon dioxide, could be carbon mono oxide, could be water, could be anything else could be nitrogen substances, may be this hexane.

I should have said normal hexane is c 12 h 14 c 6 into 2 into 14 h 14. Let us say h 14 plus air is products here and therefore, what is it we are talking off. You know we must remember see we must we talk, we cannot talk in terms of units of mass. We say when for his particular reaction, we say well one mole of hexane reacts with one mole of air to form. Let us say one more of products, one into this, one into this, one of this, but therefore, in a chemical reaction, we use the terminology moles.

What is this mole why do not we use the unit of mass why do not we say so much kilogram reacts with so much kilo gram to create products which are so much kilograms. It is possible to use, but what is this mole, let us first introduce the concept of mole because when we see rate of reaction we will again see mole is not the apt term to use. May be we should use something like concentration, but what do we mean by mole. You know we let us put things more clearly whenever we say mole, what is it we mean. You know we have quantity of matter. Let us say I have some amount of hydrogen.

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Let us say I have something like 4 grams of hydrogen with me in a particular bottle. That means I have a certain quantity of hydrogen and how do we define mass. Mass is the quantity of matter in a particular body. Therefore, when we say yes mass we mean quantity of matter quantity. Well, you know when we say mole it also talks of the same thing, it also talks in terms of quantity of matter, but instead of talking in terms of kilograms or grams we say in terms of molecular mass.

What does this mean, supposing we say hydrogen has a molecular mass and we know molecular mass of hydrogen is 2 grams per mole. Therefore, to describe the quantity of matter of contain 4 grams of hydrogen I just tell myself the number of moles of hydrogen is 4 grams divided by 2 grams per mole, which is equal to 2 moles. Therefore, mole is also a unit which describes the quantity of matter. Well you know I go to the market, I want to buy let us say one kg of potato. You know I need not, the quantity I want to buy is one kg, if I knew if I say that the molecular mass of potato is something like 2000 gram per mole.

I can as well tell the shopkeeper may be if he is smart he will understand it I can say I need to buy 1000 divided by 2000 moles of potato which is equal to 0.5 moles of potato. Therefore, all what I am saying is moles is just a unit of the quantity of matter in a substance and this quantity moles, helps us to write the chemical reactions and it is a useful tool while studying chemistry of substances. Therefore, we will in in the course of today's lecture and next 2 or 3 lectures confine ourselves in describing the quantity of a substance in terms of moles.

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We will also see in terms of volume, in terms of math, but what we do is let us say moles by now the definition of moles must be clear. Let us say I have a reaction just to make sure we understand it, in which may be hydrogen reacts with oxygen to from, let us say oxygen, oxygen molecule to form, let us say water. I tell well this equation is not balanced, I just wrote hydrogen reacts with oxygen to form water.

Now, in this reaction I say 4 grams of hydrogen reacts with let us say some substance may be 32 grams of hydrogen to form let us say 32 mass must be concerned, it forms 36 grams of water 32 grams of oxygen to form 36 grams of water because mass has to be conserved. Now, how do we write this equation, well if in terms of moles I have 4 divided by 2 gram per mole, that is 2 moles of hydrogen.

I have 32 I have 32 oxygen is 32 grams per mole that is one mole of oxygen. I have 36 grams of water, 36 and h 2 o has a molecular mass of 2 plus 16 that is 18 grams per mole that means 2 moles. Therefore, this equation I can write 2 h 2 plus I have 1 mole that is 1 of o 2 gives me something like 36 divided by 2 that is 2 moles of water. This is how we write a chemical reaction, that means we write in terms of moles. This moles as an advantage you know it is much easier to use than to write a chemical reaction in terms of moles, rather than to write in terms of masses. We will use this unit of moles while talking in terms of chemical reaction. Now, from when we talk of moles, it is also necessary to distinguish the word mole from molecules.

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You know when we say molecules, you know we have any substances and any substance let us say I have a quantity of a substance over here. It contains of lot of molecules small small molecules which are interacting with each other in the substance. Therefore, one particular mole, if I say one mole of a substance it contains the Avogadro's number of the molecule that is 6.023 in to 10 to the power 23 molecules.

Let us not confuse the word between molecules and moles. Well 1 mole consists 6.023 in to 10 to the power 23 molecules which is known as Avogadro's number. You know there is one great advantage in working with moles, if we consider in terms of a gas let us consider an ideal gas, we say well an ideal gas is described with the equation p v is equal to mass in to specific gas constant into temperature if we want to express instead of moles instead of mass over here. So, much kilogram specific gas constant is in Jules per kilogram kelvin.

Supposing, I were to write in terms of moles. Therefore, I can write this equation p v is equal to the number of moles in to the universal gas constant r naught into t where r naught is the same for all gases and it is equal to 8.314 Jule per mole kelvin. Therefore, I do not need to go back and find out the specific gas constant for each gas and then relate the mass and the volume, rather if I write in terms of moles I have I can use the gas constant that, is the universal gas constant to relate volume and temperature with respect to the moles over here.

Therefore, form this definition it also works out, if I consider the standard temperature and pressure conditions, namely one atmosphere pressure may be a temperature of 25 degrees centigrade which we call standard temperature and pressure. If I were to say what is the volume occupied by one mole that means v is equal to volume occupied by one mole over here into r naught 8.314 Jule per mole kelvin into temperature 25 degrees centigrade plus 273 298 divided by something like pressure comes over here.

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Pressure is one atmosphere that is 10 to the power 5 Pascal. Well the volume which comes out to be equal to 0.0224 meter cube. That means the volume occupied by one mole of a gas at of any gas at standard temperature and pressure there is something like 22.4 liters and these things will be useful for us when we do the calculation. Therefore, to begin with discussing about energy release, we talk we must first be very clear that we will like to use the terminology moles instead of may be mass.

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Instead of describing the quantity of a substance as meter cube we will like to use moles for description. Having said that let us go forward. Let us try to see, why should energy be released in a reaction. You know we tell ourselves well what did we say, I have let us n 1 moles of a fuel with n 2 moles of an oxidizer, let us say oxidizer I do not know what this oxidizer is, could be oxygen it could be chlorine it could be any other oxidizer.



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Let us say it forms n 3 moles of some products. I am interested in finding out what is the energy released. Now, this has fuel and oxidizer therefore, it becomes something like an explosive. I want to find out how much energy is released in this particular reaction. Therefore, what is it I do, well I realize if energy has to be released you know this substance has some energy by itself.

You know any substance, like I take this piece of duster which is wood. Well wood also contains carbon, hydrogen, oxygen stuff like that. It also contains some energy some in aid energy some internal energy and therefore, we say well any fuel substance will contain some inherent energy and where does this inherent energy come from. Well it has all these bonds which are there, may be you have all these bonds of carbon, hydrogen oxygen or whatever it is it has.

All these structure and it has some energy which we could call as internal chemical energy. Let us call it as I C E internal chemical energy. So, also when I consider that means n 1 of fuel has certain amount of internal chemical energy. The n 2 moles of oxidizer has also some amount of energy which I call as corresponding to oxidizer. This corresponds to fuel over here.

Then the products you know when I react fuel with oxidizer I get different structure. Well it could also this could also contain some internal chemical energy. Let us say of product, now if I look at the structure and find well the internal chemical energy of products, let us say is 200 some units for the total of the n 3 moles. If the internal chemical energy of the oxidizer is let us say 50 Jules over here, for the total here it is 200 Jules for the products over here.

If for the fuel it is let us say 120 Jules over here. The total internal chemical energy of the fuel and oxidizer in this particular, for these particular moles is 170 Jules. In this case well my internal chemical energies 200 Jules which means well energy cannot be liberated in this. Only what is happening for this reaction to go on I must supply some energy which is equal to 30 Jules. Such that I get the net energy because energy is conserved energy cannot just be picked up and it is something which is conserved in a chemical reaction or in in universe.

Maybe we say well that is the first law of thermo dynamics energy is conserved. Therefore, we say for this reaction to take place I must supply some energy, but supposing the internal chemical energy of the products where something like let us say 100 Jules, then what is happening. The internal chemical energy of the reactants that is the fuel and oxidizer was something, let us say I put energy on this scale. Well I put a time scale over here, time scale over here let us say T.

Initially I have substances which are just reactive the total energy was 170 afterwards when things got completed well the energy is something like 100 over here. Therefore, I get this energy which is released and this is the energy form the chemical reaction. Therefore, we find that when the internal chemical energy of the total products is less than the internal chemical energy of the substances, which react or reactants which we call. If this is less than this well some energy is released. Therefore, I can write the energy release in a chemical reaction.

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That means let us say energy release in any chemical reaction e naught or e is equal to internal chemical energy of all the products put together for all the moles which are formed, minus the internal chemical energy of the reactants over here. To be able to deliver energy, well it must decrease or rather energy in Jules is given by negative of I C E for the products, minus the internal chemical energy at the reactors.

Well this is how we should do therefore, we must be able to find out what is the internal chemical energy and a terminology what is used to denote the internal chemical energy, is what we call as a heat of formation. That means you know we would like to use terminologies which are more capable of being defined properly. Therefore, we say a substance is characterized in terms of heat of formation. I will say well I call this as delta enthalpy of formation at some condition, we will say call it as heat of formation.

How do I define, well it implies something like the internal chemical energy and how do I define it. Well I say heat of formation of a substance is the heat required, let us put it down heat required to form one mole of a substance from or one mole of a substance at standard condition. That means at one atmosphere pressure and 25 degrees centigrade that means the heat required to form one mole of a substance at one atmosphere pressure and 25 degrees centigrade and 25 degree centigrade from it is naturally occurring elements.

Again at one atmosphere and 25 degrees centigrade therefore, we define heat of formation as the heat required to form one mole of a substance at the standard conditions

from it is naturally occurring elements, again at the same standard conditions. Therefore, the notation is the additional heat which is required for forming a substance at the standard conditions, when the elements or the naturally occurring elements are again at the standard condition.

Therefore, this is way and this is same as the internal chemical energy let us therefore, say we can therefore, now say well the energy liberated in a chemical reaction is equal to the net heat of formation of the total products, minus let us say products minus the net heat of formation of the reactants for all the molecules, you put to the all the moles you put together you get the energy release in a reaction. We say in this reaction so much Jules is formed. Therefore, I think we must take some examples of how we define heat of formation and what is done is. It is defined with respect to the naturally occurring elements and what are these naturally occurring elements. Let us put some of them down over here.

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You know, for instance in nature, oxygen occurs as a gas, may be nitrogen is available as a gas, may be carbon is available as coal or char coal, may be carbon as a solid oxygen as a gas may be nitrogen as a gas and so on different types of elements occurring in nature. Supposing, I want to form let us say nitrogen, I could also have hydrogen as a gas which occurs in nature. Therefore, if I am interested in forming water and I want to define what is the heat of formation of water, then I am interested in forming water, but water I cannot say one atmosphere pressure.

I just say if I want to form water at 25 degrees centigrade from it is elements, namely hydrogen gas which occurs in nature oxygen gas which occurs in nature or rather h 2 as a gas at one atmosphere pressure and 25 degree centigrade, oxygen as a gas at one atmosphere pressure and 25 degree centigrade. I found water that means water as a liquid at 25 degrees centigrade. The heat required to form water from hydrogen and oxygen again at the same condition as water which is formed is what we call as heat of formation of water h 2 o liquid.

Therefore, let us take a look and by varied definition, since we are defining a substance in terms of elements. The heat of formation of the elements are 0 therefore, heat of formation of an element like let us say hydrogen gas at the standard condition one atmosphere pressure and 25 degrees centigrade is 0. The heat of formation of let us say oxygen gas at this standard condition is 0. Therefore, all these elements let us say carbon, carbon exists as a solid heat of formation of carbon at this standard condition is 0.

We have to evaluate the heat of formation as the heat required to form one mole of water from it is elements, namely hydrogen and oxygen is what is called heat of formation of water. Therefore, let us try to evaluate this we need to go and build up a table of heat of formation and it is a given. It is all these things are available as tables, but we must know how it comes from. Let us take an example, we take the example of let us say carbon dioxide I want to form let us say the heat of formation of carbon dioxide.

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We tell ourselves, well this is a substance carbon dioxide. Therefore, I have carbon as a solid and it reacts with oxygen as a gas. Let us say I found carbon dioxide as a gas therefore, I am interested in heat of formation of carbon dioxide. Well I know well these are elements I need to do this, but I also know if I take one kilogram of carbon that means I take one kilogram of carbon, I burn it in oxygen or air or whatever it is. I burn one kilogram of carbon the heat which is generated in this particular reaction is something like 32800 kilo Jules.

That means if I burn one kilogram of carbon with oxygen to form carbon dioxide the energy liberated is 32800 kilo Jules. Therefore, if instead of having that means now I say one mole of carbon if I were to burn with oxygen that means if I take this particular reaction. According to this reaction one mole of solid carbon reacts with one mole of oxygen to form one mole of carbon dioxide. Therefore, if I consider one mole of carbon well I know the molecular mass of carbon is something like 12 grams per mole.

Therefore, if I say 32800 kilo Jules is produced form one kilogram of carbon. Form one mole of carbon the amount of energy which is generated is 32800 from 12 that means into 0.012 is the amount that means per mole of carbon. This is the amount of energy which is generated which is equal to I get a value around 396 or 393.6 kilo Jules that means to generate one mole of carbon dioxide I need to supply something like 3. When I from this automatically in this reaction 393 kilo Jules of heat is getting generated.

Therefore, what does this heat do, it increases the temperature of carbon dioxide to a high value because heat is getting generated. Therefore, the gases are at high temperature, but mind you when I talk of heat of formation, I am talking of heat of formation of carbon dioxide at one atmosphere pressure and at a temperature of 25 degrees centigrade. This is the standard condition and therefore, I have to cool this gas that means the hot gas has to be cool. Therefore, when I react carbon with oxygen so much heat is getting generated.

I have to remove so much of heat to bring back the carbon dioxide to it is natural condition. Therefore, in this particular reaction I have to subtract something like 393.6 kilo Jules of energy to be able to get back the carbon dioxide in standard condition. Therefore, since I remove the heat I say the heat of formation of carbon dioxide is equal to minus 393.6 kilo Jules and this is how the values are calculated. May be you react the elements together form the substances.

If the substances generate heat well the temperature goes up I have to remove the heat to be able to get back the substance to the original condition. We say heat of formation of carbon dioxide is 393.6 kilo Jules. Let us take one more example, we take a simpler example of something like hydrogen and oxygen being burnt to form water. Well we do the same thing, but it is not as simple as that you know we have apportion things together. Let us say I am interested in heat of formation of let us say water. Therefore, I know well hydrogen as a gas one mole of hydrogen gas plus half mole of oxygen gas forms one mole of water that means as a liquid water.

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Now, what is it I am not talking off. Well if I do an experiment and in my experiment I have something like let us say I have 2 grams of hydrogen I burn with something like here 32, 16 grams of oxygen. I know that the heat which is generated in this reaction again it is an exothermic reaction. Heat is getting evolved that means I generate something like 286 kilo Jules of heat gets generated in this particular reaction or rather when one mole of hydrogen gets consumed because one mole of hydrogen corresponds to 2 gram.

In this reaction I talking in terms of 2 grams that means for every one mole of hydrogen getting consumed I generate 286 or rather when one mole water is being formed, I have an energy which is 286. If this has to be brought back to the ambient condition that is the standard condition of one atmosphere pressure and 25 degree centigrade. I have to subtract or remove the heat. Therefore, I tell the heat of formation of water as a liquid is equal to minus 286 kilo Jules per mole.

So, we can keep on doing this exercise for the different substances and let us put down list of tables and then qualify further. You know normally these things are arrived at experimentally we look at the elements in as much as they form a substance. If the reaction is exothermic well I have to remove the heat to be able to form this substance at the standard condition. If it is endothermic well I have to supply the heat and in which case the heat of formation would be positive. If I put some of the values down let us put a few values down, such that we get a feel for how to use it in case of chemical reactions.

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Let us put a few of them together. Let us say I have methane c h 4. The heat of formation of methane is minus 74.9 kilo Jule per mole. Therefore, we are talking in terms of energy per mole. I take form methane I go to ethane c 2 h 6. The energy or heat of formation is equal to minus 84.7 kilo Jule per mole, I go to propane c 3 h 8, the heat of formation is minus 100 and 3.9 kilo Jule per mole. I come to the last category, you know this are all alkenes methane, ethane, propane may butane c 4 h 10 and so on it goes.

We will stop with this hydro carbon chains with this minus 124.7 kilo Jules per mole. If I take a more longer chain, like I say kerosene which is something like dodecane. Dodecane means c 12 h 26 which is kerosene. The heat of formation is higher at minus 292.9 kilo Jules per mole. How do I determine all this? Well we just now told ourselves well I will react carbon at the standard condition of 25 degrees centigrade with let us say hydrogen gas at one atmosphere pressure and 25 degree centigrade.

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May be depending if I want methane one with 2 moles of this to form c h 4 over here, I found one mole of this I find well if heat is liberated in this reaction well have to subtract it to be able to form this. Therefore, I get minus 74.9, if I want to form something like c n h m over here well I have n of c solid plus m of h m by 2 of h 2 gives me c of n into h m which for which I can do this particular reaction or a combination of reactions and find out the heat of emission.

This is how it is done and these are the values which are reported in literature. Let us take a one or two more substances. Well we take acetylene and what is the difference see these are all alkenes, this is alkyl acetylene is  $c \ 2 \ h \ 2$  and the structure of these substances were quite simple. We have  $c \ h \ 4$  we have  $c \ c \ h \ 6$  over here, these are the hydrogen atoms which are attached to this. We have  $c \ 3 \ h \ 8$  we have hydrogen bonded to this so on, but when it came to acetylene, we had something like a triple bond.

Then we had h and h over here c 2 h 2 and in case of acetylene the heat of formation is positive and it is equal to plus 226.7. Well what is it we see form this tables we will just take a look at this and proceed with heat of formation of one or two more substances. We find as the substance increases in complexity that means as the bonds keep on increasing. Well the heat of formation becomes more and more negative that means may be kerosene is has a much more much higher value, but it is a more negative value than may be methane.

We also find as the molecule becomes more complex, this is a gas, this is a gas, this is a gas, but it liquefies a little earlier. Well this becomes a volatile liquid may be as a substance increases in complexity it also from a gas phase it also exists as may be a kerosene liquid. I go to naphthalene and naphtha which are exist as solids and therefore, we see that as a substance becomes more complex well the heat of formation becomes more negative, but as a higher value.

In the case of acetylene which is a triple bond, well I have to supply heat that means compared to kerosene which reaction to form kerosene I generate heat I ways I have to supply heat therefore, lot of heat gets locked into it. Therefore, you know acetylene is a gas which is used in welding, but it is it is quite strong I can release it is energy spontaneously. It is a very strong explosive may be we will take a look at this a little later. Let us put down one or two more values of heat of formation before I go back and learn how to apply it and also we see what is the meaning of all these things. Let us take 2 more substances well I have water.

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$$BH_{1}^{o} = -2867 \frac{k_{T}}{mde}$$

$$BH_{1}^{o} = -110.5 \frac{k_{T}}{mde}$$

$$\Delta H_{1}^{o} = -3935 \frac{k_{T}}{mde}$$

I have heat of formation of water, we just now were telling x equal to minus 286. 7 kilo Jules mole. Heat of formation of carbon dioxide at the standard condition mind you solve standard condition is equal to minus 110.5 kilo Jule per mole and heat of formation of carbon dioxide is equal to minus 393.5. Therefore, these are these things which are available in literature and how do we do, we do in experiments in which we find whether

heat is generated while forming these substances from the naturally occurring elements. Then we put this values down, but it is also possible to calculate these things and why do we say that.

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When we talk of the internal chemical energy of a substance, what is it. We mean we mean the energy associated with the particular structure we say methane has these particular bonds in which carbon is associated with the bond over here. Therefore, it is possible to express the heat of formation in terms of the bond energy or the structure, the energy of the structure of the particular molecule. Therefore, let us say I am interested in heat of formation of water.

If I want to find the heat of formation of water well water is h 2 o it consist of o h and h it consists of 2 o h bonds. How is water formed well I consider the hydrogen molecule which has h h bond. I have half a mole of oxygen, one mole of oxygen has this particular bond and what is it I form I form 2 o h bonds over here as water. Therefore, if I were to determine the heat of formation of water see I define heat of formation as the heat required to form one mole of a substance at standard conditions.

From this elements again at standard conditions and therefore, now you know I put some energy here I put some energy here. That means the heat of formation I have to bring these things back to the day time value or rather I must be able to write heat of formation of the product, which is water here is equal to the bond energy what is available to me for the structure.

That means I have m 2 of the o h bonds are available minus I have the energy that is the bond energy of h h atom plus I have half a mole. That means half bond energy of this particular one. You know these bond energies of may be a oh bond may be h h bond may be the o o bond are all available in literature. These chemists have determined the values of these bonds and let us take some values. You know if I take the value of the hydrogen bond. The o h bond has an energy of 464 kilo Jule mole the h h bond has an energy of 436 whereas, the o o bond has an energy of 499.

Therefore, if I take a look at heat of formation in terms of difference in bond energy, what is it I get the heat of formation can be calculated formed these bond energies as equal to I have 2 o h bonds that is 2 into 464 minus. I have one h h bond that means equal to into the value of 464 and I have half of this. That means plus u have 499 divided by 2 and this is the heat of formation.

Therefore, what is happening is therefore, I will get the heat of formation of h 2 o, but you know when the bonds are being formed the water is the hydrogen is a gas, the oxygen is a gas we are talking of heat of formation of water as the gas. Therefore, I also have this gas has to be converted to a liquid therefore, I have to add the latent heat of water which is equal to let us say h per mole of vapor to liquid. The value is something like 45 kilo Jule per mole is the latent heat of vaporization plus.

I also want to bring down the water to one to bring down the water at 100 degree centigrade at atmospheric pressure to 25 degrees. Therefore, I have c p into something like from 100 degree centigrade I have to reduce it to 25 degrees centigrade. If I put all these things together, I will get the heat of formation of water to be given by something like minus 280 or so, but you know we must remember calculating form bond energies is not very correct because it is not only the bind energy which exists for a particular molecule, but a molecule will also have vibrational energy.

It could have resonance energy and so on and, but what we do is, we use the values which are available in literature, but all what I wanted to tell was heat of formation being the internal chemical energy of a substance can also be derived from the bond energy. Well we now know how to calculate the bond energies rather the heat of formation. Now, we can calculate the heat released in any chemical reaction. So, or let us put that together for one particular problem.

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Supposing I say a given volume, let us say one meter cube of butane gas c 4 h 10. This butane gas one meter cube also is mixed with air in some proportion and when chemical reactions occur between that is I have one meter cube of butane gas and air mixed together. They form products which are let us say c o 2 and some of that substances. Well I have carbon dioxide which could be formed, I have water which could be formed. Supposing, these are the 2 substances which are formed.

I presume they are formed we must be able to calculate them as we go along I presume that these are the substances which are formed. I want to calculate how much energy is liberated from this particular volume. This is what I will do to begin within the next class. Then we will go ahead and try to find out how to fix the products which are formed. We will define something like a stoichiometry coefficient, we will also talk in terms of fuel rich and oxidizer rich mixture which is being formed. For these conditions how to calculate the products and then how to calculate the energy release in a chemical reaction.

Well, thank you.