Let’s take a look at this reaction between propane and oxygen. Well, that was a pretty dramatic explosion! And I can pose the question: Is there any way we could have predicted that that’s what was going to happen? Again, it was a reaction of propane and oxygen. The answer is that we have a very powerful tool for making predictions about the thermochemical outcome of chemical reactions, and that tool is the fact that we can measure and tabulate average bond energies.

Here’s the idea. We have these tables of average bond energies that I’ve shown you before. These are the multiple bond average bond energies. Remember, these are the amounts of energy in kilojoules that you have to put in in order to break a mole of the bond. To break a mole of N-N double bonds you have to put 418 kilojoules in, and similarly, here are the numbers for single bonds. Now these, remember, represent average bond energies. In other words, on average, if we have a nitrogen-oxygen single bond, we’d have to put in 201 kilojoules to break a mole of those bonds.

The reason why they’re useful is because we can then use them to predict enthalpies of reaction based on these average bond energies. Now, it’s going to be a back-of-the-envelope calculation. It isn’t going to be exact, and the reason why it’s not exact is because the average bond energies represent averages. But let’s take a look at the reaction that we just saw anyway. Here’s propane, . To balance this reaction and give carbon dioxide and water, we have to add five oxygen molecules, and it gives us three carbon dioxides and four waters. Now, one thing that’s important is that these are all in the gas phase, and these calculations only work when the reactants and products are all in the gas phase, because bond association energies are gas phase measurements. We can’t talk about making water liquid here or using a liquid fuel here. It’s got to be gas and gas going to gas and gas.

If we write out Lewis dot structures for these molecules—and I’ve left off the lone pairs, but don’t worry about it—you can at least in your mind imagine that we’re taking a mole of propane and five moles of and going to three moles of carbon dioxide and four moles of water. What we’re going to do is dissect each of these molecules by breaking the bonds that are present. For instance, to dissect propane into its constituent atoms, we would have to break two carbon-carbon bonds and eight carbon-hydrogen bonds. Similarly, to break up three moles of , we would have to break six moles of carbon-oxygen double bonds. And that’s illustrated on the next page.

What we have here is we’re starting with propane and five moles of , and this is the level of our reactants. I just drew the line here arbitrarily at this point on the page because it fit. Remember, energies are relative, so it doesn’t really matter where I draw the purple line. However, relative to these molecules, if I put in an amount of energy that breaks all the carbon-hydrogen bonds and all the carbon-carbon bonds and all the oxygen-oxygen bonds, we have to break eight carbon-hydrogen bonds, so eight times the average bond energy of a carbon-hydrogen bond, which is 413 kilojoules—right off the table, just read it off the table. Two carbon-carbon bonds, or the dissociation energy of a carbon-carbon bond, times two because we have to break two moles of those bonds, plus five moles of oxygen-oxygen bonds. Those are double bonds, 498, and you have to make sure you look at the oxygen-oxygen double bond value, not the single bond value. If we put that amount of energy in, we’re going to get all the way up to atoms. So this is not 100. This is 10 oxygen atoms. So three carbon atoms plus eight hydrogen atoms plus 10 oxygen atoms, and that’s our constituent atoms from our reactants. We add all that up, and we would have to put in at least our thought process—remember, this is a Hess’s law kind of problem—6,486 kilojoules to break up one mole of propane and five moles of .

And now let’s take these atoms and reassemble them into our product molecules. We’ll make six moles of carbon dioxide bonds, a total of three carbon dioxide molecules but six moles of bonds, so it’s 6 times 732, which is the carbon-oxygen bond energy. You’ll notice that there’s a minus sign here. Why is there a minus sign? Because these were energies we had to put in; hence the positive quantity. Remember, endothermic processes are positive. But now we’re getting energy back out, and it’s the negative of the bond association energy, so there’s a negative here. And then after that, eight moles of O-H bonds, 8 times 463, which is the association energy of the oxygen-hydrogen bond. So we add these two quantities together, and it gets us to –8,096 kilojoules.

What this says is, roughly speaking, if we take a mole of propane and five moles of and react them to form three moles of carbon dioxide and four moles of water, the reaction is exothermic by the difference in the energies between reactants and products, which is this number plus this number. And this number plus this number is equal to this value.
right here, from this red line down that red line, which is -1,610 kilojoules. The reaction is exothermic. In other words, we had to go up a certain amount, we come back down a certain amount, and since we ended up with products lower than reactants, the reaction is exothermic, and it's by this amount: 1,610 kilojoules. Now this is, again, an approximation, because these D values are all approximate. They're all average bond values.

Let's now look at how close we came to the real number based on real thermochemical data—in other words, based on heats of formation or enthalpies of formation. Remember, the standard enthalpy of reaction is equal to the sum of the standard enthalpies of formation for products minus reactants. We have among the products four moles of water (so four times the standard enthalpy of formation of water gas) plus three times the standard enthalpy of formation of gas, minus—here’s the reactants—there's propane and then there is oxygen. We look these numbers up in a table as well. That’s the number for water. That’s the number for carbon dioxide. That’s the number for propane. Recall that the standard enthalpy of formation for is zero because this is an element in its standard state. We work through this math, and we get -2,043.9 kilojoules. If we compare this number to the number that we saw before, which was 1,610, we can see that we’re within 20% or so of the true thermochemical value. This is a back-of-the-envelope estimation, but it's pretty good, considering we were using tables of data that are encompassing all different kinds of carbon-oxygen bonds and oxygen-oxygen bonds.

Why are these useful? Well, sometimes you don’t have these enthalpies of formations for everything that's in your reaction or everything that's in your product. So this equation is not useful if you don’t have these enthalpies of formation, but you can almost always dissect your molecule into the constituent bonds, of which there are just a few, and that allows you to do these calculations to get an idea of how your reaction is going to proceed, whether it's going to be endothermic or exothermic.

Now, one last thing is that you can see that this difference here between reactants and products gets larger as these starting materials move up in energy. What does it mean for them to be moving up in energy? The answer is: they have weaker bonds. As they have weaker bonds, it takes less energy to break it up into atoms. So if you do the calculations, what you’d find is, molecules that are good explosives are molecules that have typically weak bonds relative to products. And products are things that have really strong bonds, things like carbon dioxide and water and . If you did this sort of calculation for nitroglycerin or trinitrotoluene or something like that, what you’d see is that this level is really high up relative to the products, and it has to do with the fact that the reactants have relatively weak bonds. Exothermic reactions are reactions in which you're trading weak bonds within the molecule for strong bonds that you’re forming in the products. So, again, what all of this exercise tells you is that you can do estimates of the thermochemical outcome of your reaction based on average bond energies.