

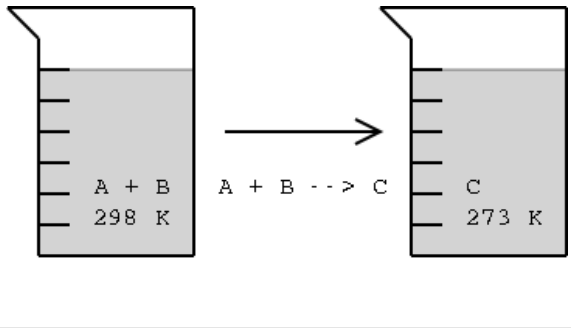
Introduction

We've discussed heat briefly, and we've stated that the heat is an energy flow between systems that differ in temperature. Since we're chemists, though, we'd like to relate all this talk about heat flows, systems, and surroundings to what we're interested in - chemical reactions. This has important practical considerations. Heat is transferred in nearly all chemical reactions, and you have to take these into account when performing reactions. Sometimes this heat is desirable - you'd have a tough time cooking your food on a gas stove if the combustion process wasn't exothermic! In other cases, the heat is a serious safety concern. The reactions used to make plastics, for example, are often extremely exothermic. These reactions, if uncontrolled, can proceed very quickly and lead to explosions. (Consider what a large temperature increase can do to the pressure in a sealed vessel!)

We will discuss what the **heat of reaction** is and how we can both measure (and predict) this quantity. We will then use it to calculate how much heat is transferred in a real chemical reaction where we have a given amount of reagent.

Heat of reaction

The **heat of reaction** is defined as the amount of energy required to bring a system back to its original temperature after a chemical reaction. Let's say we have a chemical reaction in a beaker. The reaction causes the temperature inside the beaker to drop.

	<ul style="list-style-type: none"> • A, B, and C are all present in aqueous solution in this example. • Why does the temperature in the beaker drop? What is removing energy from the contents of the beaker? • Define the system as the substances involved in the chemical reaction, and the surroundings as the beaker of water.
<p>Illustration 1: Temperature change in a chemical reaction</p>	

In the above illustration, the beaker's contents are cooled. But by what? The only apparent source of the cooling would be the reaction of A and B to form C. The formation of C is an **endothermic** process (and the reaction is said to be an **endothermic reaction**) - C has more **internal energy** than the starting materials.

Energy flows from the water in the beaker to the reacting substances. This loss of energy from the water causes its temperature of the water to drop. The reacting substances accept this flow of energy and use it to complete the chemical reaction. Since energy flows **into** the system (the reaction), the measured Q (the **heat of reaction**) for this system it would be **positive**.

How you'd report a heat of reaction to others

The energy absorbed or given off by a chemical reaction depends on the amount of reactants present. The more moles of chemicals react, the greater the heat transfer (in either direction). So it's not terribly useful to say something like "I did a reaction between A and B to get C and the heat of reaction (the Q) was 236.7 kJ." You've told your listener that the reaction was endothermic (because Q was positive), but you really haven't said much else. The number you've given is meaningless without some description of how much C you actually made, or how much A and B were reacted. Because of this, heat of reaction is typically expressed as energy units **per mole** of a substance involved in the reaction.

We don't normally report values of Q for chemical reactions. Instead, we report what is called the **enthalpy change of reaction** (often just called **enthalpy of reaction**). Without going too deeply into the math and language of thermodynamics, we will say that there are several reasons that we express reaction heats in terms of this **enthalpy**.

1. **Enthalpy** is a mathematical construct, abbreviated as **H**. You can think of it as measuring the most efficient path from products to reactants. Consider the energy content of the products and the energy content of the reactants as two locations in South Carolina - say, Florence and Columbia. If you drive a Honda Civic to Columbia from here and someone else drive a Jeep Cherokee, you'll expend different amounts of energy, but you'll both arrive in the same place. You can think of the enthalpy as the **idealized energy change between products and reactants**.
2. **Enthalpy** is constructed so that the **enthalpy change for a reaction** is equal to the **heat change at constant pressure**. Since we normally do chemical reactions in our lab at these conditions anyway (in a beaker on the desk, for example), enthalpy change is easy to measure. Someone who's taken a thermodynamics class or two can take that enthalpy change and use it to deal with other conditions.
3. **Enthalpy** is **related to internal energy**, which is the concept we discussed earlier. It is defined as $H = U + PV$, where P and V are pressure and volume.
4. **Enthalpy** is a **state function**. This means that the enthalpy content of a substance at a given set of conditions is the same no matter how the substance got to those conditions. The amount of heat you measure from a reaction may depend on how you performed the reaction - since energy takes forms other than heat, but the enthalpy change is always the same.

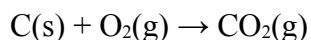
Enthalpy is a property of a substance. Heat, however, is an energy transfer. The heat of a reaction, then, is related to the enthalpy **change** between the products and reactants. You'd calculate this enthalpy change like this:

$$\Delta H_r = \frac{Q_{\text{reaction}}}{\text{Number of moles}}$$

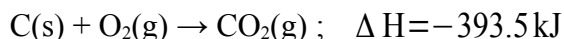
where ΔH_r is the enthalpy change of the reaction (abbreviated as the **enthalpy of reaction**, and often just called the heat of reaction) and Q_{reaction} is the heat change of the reaction measured at constant pressure. We will measure the enthalpy change of some reactions in the lab.

The thermochemical equation: Another way to express reaction heats

Another useful (and unambiguous) way to express a heat of reaction is by the use of a **thermochemical equation**. A thermochemical equation is just a chemical equation with added heat data. For example, let's look at the chemical equation for the combustion of graphite (a common form of carbon):



This is the chemical equation. A **thermochemical** equation contains the same information plus the heat of reaction **as the reaction is written**. For the combustion of graphite:



Some important things about the **thermochemical equation** are:

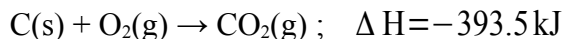
- The enthalpy change (or heat) given is for the equation **as written**. In the example, 393.5 kJ of heat are released if 1 mole C solid reacts with 1 mole O₂ gas to form 1 mole CO₂ gas.
- Phase labels are **required**, because phase changes involve energy. For example, production of **liquid** water involves a different amount of heat than the production of **gaseous** water or **solid** water. The same is true for any other substance.

You can modify thermochemical equations much like you'd modify chemical equations. There are **two important modifications** you should be familiar with.

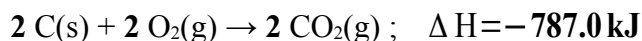
1. You can multiply a thermochemical equation by a factor. When you do so, you also multiply the enthalpy by the same factor. It's like the heat is simply another product of the reaction.

For example, what if you were interested in the heat given off by the burning of **two**

moles of graphite? Well, you'd just multiply the reaction by two, just like we you scaled up chemical "recipes" (equations) earlier.



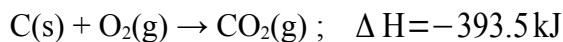
becomes



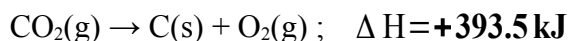
So, two moles of graphite releases 787.0 kJ of heat when it is burned.

2. You can reverse a chemical reaction by switching products and reactants. If you do that, you must change the sign on the enthalpy. This should make logical sense. If a combustion, for example, releases energy, you would have to re-add that energy to get the original materials back.

For example, let's see how much energy would be required to convert a mole of carbon dioxide back into carbon and oxygen.. We know:



Reversing, we get



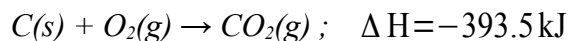
So, it would require 393.5 kJ of energy to split carbon dioxide into graphite and molecular oxygen. (*Though this reaction is theoretically possible with the right application of energy, this isn't a very **practical** way to get graphite.*)

Application: Heat production or requirement in real reactions

As we said in the beginning, these heats of reaction (or enthalpies of reaction) are useful to us because they provide practical information like how much heat we need to supply to make a reaction go or how much heat we can expect a reaction to produce for us.

It shouldn't be a surprise to you that we can use these heats to simply calculate how much heat is produced when a given amount of reagents reacts, or to calculate how much of a reagent is necessary to supply a required amount of heat. For example, let's go back to burning graphite.

How much heat is produced when 2.524 grams of carbon are burned in the presence of oxygen? The thermochemical equation is:



This is a stoichiometry problem, You can treat the heat just like it is another product. To solve it, first we **calculate the number of moles of carbon**, then we **relate the moles of carbon to kilojoules of heat using the thermochemical equation**. This is similar to finding the moles of product produced in a simple stoichiometry problem.

Find the moles carbon:

$$2.524 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 0.2102 \text{ mol C}$$

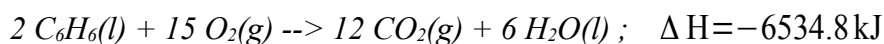
Now, find the amount of heat using the thermochemical equation. As long as the reaction takes place at constant pressure, the heat production will be the same as the enthalpy change:

$$0.2102 \text{ mol C} \times \frac{-393.5 \text{ kJ}}{1 \text{ mol C}} = -\mathbf{82.71 \text{ kJ}}$$

We've calculated the value of Q for this reaction. Q is negative, so the reaction is **exothermic** (it gives off heat, just as we'd expect from a combustion). To put it in plain English, **82.71 kJ of heat is released by the burning of 2.524 g of graphite.**

Let's look at another problem, this time trying to figure out how much of a material it takes to generate a desired amount of heat.

How many kilograms of benzene (C₆H₆, FW = 78.11 g/mol) must be burned to produce 150000 kJ of heat? [Calculate your answer to four significant figures.]



We have an amount of heat we'd like to produce this time and are asked how much reactant we need to consume to produce it. This problem is worked just like you'd work a stoichiometry problem where you were asked how much of a reactant you'd need to produce an amount of a desired product. Again, the heat is just like another product!

First, we calculate the **number of moles benzene** required to produce the given heat, assuming the reaction takes place at constant pressure. We use **the thermochemical equation** to get the conversion factor. Then we calculate the mass of benzene required from the formula weight.

"Producing" heat means that the sign of Q is negative, so ...

$$-150000 \text{ kJ} \times \frac{2 \text{ mol C}_6\text{H}_6}{-6534.8 \text{ kJ}} = 45.91 \text{ mol C}_6\text{H}_6 \text{ required}$$

Now, we calculate the mass (remember, the problem specifies **kilograms**).

$$45.91 \text{ mol C}_6\text{H}_6 \times \frac{78.11 \text{ g C}_6\text{H}_6}{\text{mol C}_6\text{H}_6} \times \frac{\text{kg}}{10^3 \text{ g}} = \mathbf{3.586 \text{ kg C}_6\text{H}_6}$$

So, you must burn **3.586 kg C₆H₆** to produce **150000 kJ of heat**.

Summary

In this note pack, we've learned the definition of the heat of reaction, the notion of a thermochemical equation, and how to use the heat of reaction and thermochemical equations to find out information about heat transfer during real chemical reactions.

In the next pack, we will talk about Hess's Law, a way to determine the heat of reaction without doing an experiment. We will also discuss how heat changes are measured.