Bond Energy

What makes a reaction endothermic or exothermic?

Why?

Chemical reactions can be a lot like playing with Legos®—you must take apart part of your last creation before you can replace it with something new. For many chemical reactions, we have to first break bonds in the reactants before we can put the atoms back into a new arrangement to form the products. Both of these processes involve changes in energy. The net energy change for a reaction is called the **heat of reaction** or the **change in enthalpy** (ΔH). In this activity we will look at one way energy changes can be approximated for chemical reactions.

Model 1 – Breaking and Forming Bonds

	Reaction	Change in Energy (kJ/mol_{rxn})
A)	$PCl_3(g) \rightarrow P(g) + 3Cl(g)$	+ 966.7
B)	$PCl_5(g) \rightarrow P(g) + 5Cl(g)$	+ 1,297.9
C)	$PF_3(g) \rightarrow P(g) + 3F(g)$	+ 1,470.4
D)	$PF_5(g) \rightarrow P(g) + 5F(g)$	+ 2,305.4

	Reaction	Change in Energy (kJ/mol_{rxn})
E)	$P(g) + 3Cl(g) \rightarrow PCl_3(g)$	– 966.7
F)	$P(g) + 5Cl(g) \rightarrow PCl_5(g)$	– 1,297.9
G)	$P(g) + 3F(g) \rightarrow PF_3(g)$	– 1,470.4
H)	$P(g) + 5F(g) \rightarrow PF_5(g)$	– 2,305.4

1. Identify four reactions in Model 1 where bonds are being broken. Write "broken" in the Change in Energy box in the table for each reaction you identify.
2. Identify four reactions in Model 1 where bonds are being formed. Write "formed" in the Change in Energy box in the table for each reaction you identify.
3. Circle the correct word to complete each sentence below.
   a. When bonds are (broken/formed) there is a positive energy change.
   b. Breaking bonds is (endothermic/exothermic).
   c. When bonds are (broken/formed) there is a negative energy change.
   d. Forming bonds is (endothermic/exothermic).
4. Find two reactions in Model 1 that are exact opposites of each other, that is, one reaction is the reverse of the other reaction.
   a. How do the changes in energy for the reverse reactions compare?
   b. Explain your answer to part *a* considering what you learned from Questions 1–3 about bond breaking and bond formation.

5. Consider the data in Model 1.

   a. What unit is on the energy changes?

   b. For Reaction A of Model 1, how many P–Cl bonds are broken with the 966.7 kJ of energy listed? *Hint:* Look at the units you listed in part *a*.

   c. Calculate the energy needed to break one mole of P–Cl bonds in Reaction A.

6. Use the data in Model 1 to answer the following questions.

   a. Calculate the energy needed to break one mole of P–Cl bonds in Reaction B.

   b. Do the P–Cl bonds in different molecules require the same amount of energy to break?

STOP

Read This!

The energies you calculated in Questions 5*c* and 6*a* above are called **bond energies**. The bond energy for a particular type of bond can vary from one molecule to another because the atomic environment of a bond can influence the amount of energy needed to break the bond. For example the carbon–carbon bond in the two molecules shown below may not have the same bond energy because the surrounding atoms are different.

Bond energies can be very useful (as you will soon discover) for calculating the net energy change in a reaction. However, a table listing the bond energies for even the most common substances would be several pages long. For this reason, chemists often approximate energy changes using *average* bond energy.

Model 2 – Average Bond Energy

Bond	Energy (kJ/mol)	Bond	Energy (kJ/mol)
H—H	432	N—N	160
C—H	411	N=O	631
N—H	386	N≡N	941
H—Cl	431	N—O	201
C—C	346	Cl—Cl	243
C—O	358	F—F	158
C—N	305	O—H	464
C—Cl	327	O—Cl	269
C=C	602	O—O	204
C=O	745	C—F	552
O=O	494	C—S	259

7. Look at the bond energies in Model 2.
   a. Are the bond energies positive or negative?

   b. Do the bond energies refer to bond-breaking or bond-forming processes?

8. Look at the energy values in Model 2.
   a. What are the units for bond energy?

   b. How many bonds will the energy listed in the table break or form?

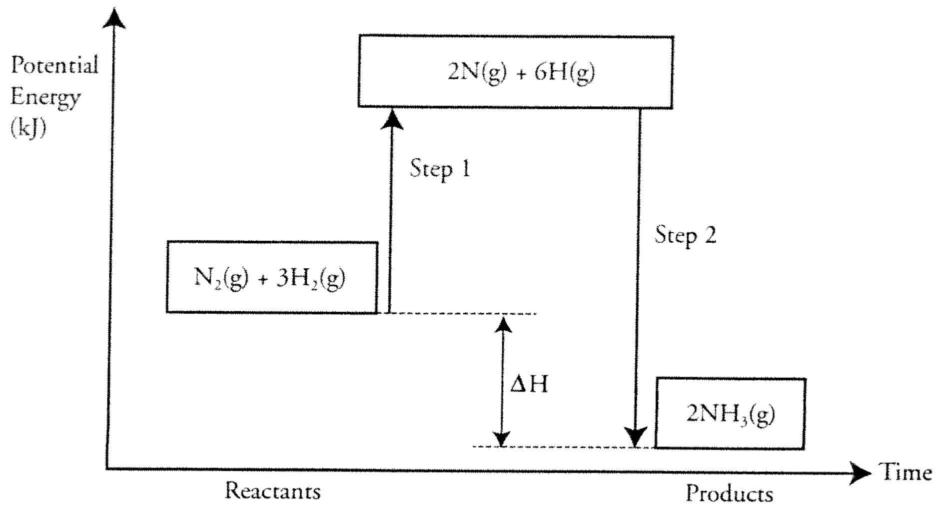
9. Is the bond energy for a double bond simply two times that of a single bond for the same atoms? Provide two specific examples to support your answer.

10. Explain how to use the information in Model 2 to determine the change in energy when a mole of C—H bonds is *formed* rather then broken.

11. Because the environment surrounding a bond in a molecule alters the bond energy slightly, predict how scientists might calculate *one* bond energy value for the table in Model 2.

STOP

Model 3 – Calculating the Net Energy Change of a Reaction



12 Write the overall reaction for the process that is illustrated in Model 3.

13. What does the *y*-axis on the graph in Model 3 represent?

14. Consider the process illustrated in Model 3.

   a. Does Step 1 represent a bond-breaking or bond-forming process?

   b. Explain why the Step 1 arrow goes up—toward higher potential energy—rather than down.

15. Draw a Lewis dot diagram for *every* reactant molecule in Model 3.

16. Use the bond energies in Model 2 to calculate the energy needed to break apart the four moles of molecules in Step 1 of the reaction in Model 3. Include the proper sign and units on your answer.

17. Draw a Lewis dot diagram for *every* product molecule in Model 3.

18. Use the bond energies in Model 2 to calculate the energy that is released to form the two moles of molecules in Step 2 of the reaction in Model 3. Include the proper sign and units on your answer.

19. The heat of reaction or change in enthalpy (ΔH) of a reaction is the net energy change in the reaction. Consider where ΔH is located in Model 3. Discuss with your group members how your answers to Questions 16 and 18 could be used to calculate the enthalpy change (ΔH) for the reaction in Model 3, and then do the calculation.

STOP

Read This!

The diagram in Model 3 suggests that the production of ammonia from its elements occurs by breaking the element molecules into single gaseous atoms and then recombining them into ammonia. In actuality, very few chemical reactions occur in this manner. In fact, the production of ammonia does not happen this way. Lucky for chemists, it doesn't really matter. Enthalpy is a state function, which means the actual process or pathway by which the reaction takes place does not affect the net energy change. Therefore, it is perfectly alright to *imagine* that the reaction occurs as illustrated in Model 3. The enthalpy change that is calculated will still approximate the real-life reaction because for a state function like enthalpy only the beginning state (reactants) and the ending state (products) must be known.

20. Balance the following reaction.

$$CH_4 + O_2 \rightarrow CO_2 + H_2O$$

21. Draw a Lewis dot diagram for *every* reactant and product molecule in the reaction in Question 20.

22. Use the average bond energy in Model 2 to calculate the change in enthalpy (ΔH) for the reaction in Question 20.

23. Why are the changes in enthalpy calculated using average bond energies considered approximate values?

Bond Energy Check for Understanding:

1. Circle the correct words to complete the sentences:
   a. The breaking of bonds is (endothermic / exothermic), and therefore has a (negative / positive) ΔH value.
   b. The forming of bonds is (endothermic / exothermic), and therefore has a (negative / positive) ΔH value.
2. Explain why it is necessary to draw Lewis dot diagrams for each molecule involved in a reaction in order to estimate the enthalpy change in the reaction using average bond energies.

3. Estimate the change in enthalpy for each of the following reactions:
   a. CH_4 (g) + 2 O_2 (g) → CO_2 (g) + 2 H_2O (g)

   b. 2 H_2O (g) → 2 H_2 (g) + O_2 (g)

   c. H_2 (g) + Cl_2 (g) → 2 HCl (g)

   d. CH_4 (g) + Cl_2 (g) → CH_3Cl (g) + HCl (g)

   e. CH_4 (g) + 2 Cl_2 (g) → CH_2Cl_2 (g) + 2 HCl (g)

Bond	**Energy (kJ/mol)**	**Bond**	**Energy (kJ/mol)**
H — H	435	H — Cl	431
C — H	414	C — Cl	331
Cl — Cl	243	O = O	502
O — H	464	C = O	730