Bond Energies

Unit: Thermochemistry (Heat)

MA Curriculum Frameworks (2016): HS-PS1-4

Mastery Objective(s): (Students will be able to…)

- Identify the bonds in molecular compounds and look up their bond energies.
- Calculate the heat produced or consumed by a reaction based on bond energy calculations.

Success Criteria:

- Bond energies have the correct sign and the correct units based on where they appear in the chemical equation.
- Heat of reaction calculated from bond energies agrees with heat of reaction calculated from heat of formation data.

Tier 2 Vocabulary: bond

Language Objectives:

- Explain how heat of reaction is calculated using bond energies.

Notes:

Ionic compounds form crystals that have straightforward ratios of cations to anions, which means it is practical to publish a table of the heats of formation of common ionic compounds and to calculate the heat of reaction from heat of formation data. Molecular compounds, however, can form long chains, and there are thousands upon thousands of common molecular compounds.

For most molecular compounds, instead of attempting to publish an exhaustive list of heat of formation data, it is much simpler to publish a table of the energy it takes to dissociate the individual bonds in molecular compounds. This way, it is possible to estimate the heat of reaction by simply adding up the energies for breaking or forming the individual bonds in a compound.

These bond energies are shown in "Table AA. Bond Dissociation Energies & Bond Lengths" in your Chemistry Reference Tables on page 518. Note that the table is "bond *dissociation* energies." This means that the numbers represent the amount of energy needed to *dissociate (break)* the bonds listed. If it takes energy (a positive number) to break a bond, that means energy is released (a negative number) when the bond is formed. This means we can use bond energies to calculate the enthalpy of formation of a compound, but we need to remember that the bond energies are negative when bonds are formed.

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Here are bond dissociation energies for some bonds commonly found in organic compounds. A more extensive list can be found in "Table AA. Bond Dissociation Energies & Bond Lengths" on page 518 of your Chemistry Reference Tables.

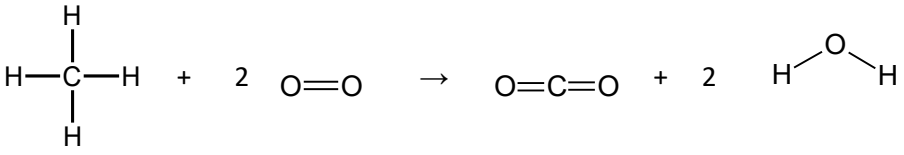
Bond	C−C	C=C	C≡C	C−H	C−O	C=O	O=O	O−H
Bond Dissociation Energy* $(\frac{kJ}{mol})$	346	602	835	411	358	799	494	459

Sample problem:

Use bond dissociation energy data to predict the energy of reaction for the combustion of methane:

$$CH_4 + 2\ O_2 \rightarrow\ CO_2 + 2\ H_2O$$

This actually means:



break 4 C−H bonds	+	2	break 1 O=O bond	→	form 2 C=O bonds	+	2	form 2 O−H bonds
4(411 kJ)	+		2(494 kJ)	→	2(−799 kJ)	+		4(−459 kJ)
1 644 kJ	+		988 kJ	→	−1 598 kJ	+		−1 836 kJ

Note that numbers on the left are positive, because we are *dissociating (breaking)* those bonds, and numbers on the right are negative because we are *forming* those bonds.

As with heat of reaction calculations, we add the energies for each of the individual molecules:

* These are bond dissociation energies are for homolytic dissociation (*i.e.,* the electrons are equally split between the two atoms). Heterolytic bond dissociation energies (where the electrons split unequally) are always higher.

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$$1\,644\text{ kJ} + 988\text{ kJ} + (-1\,598\text{ kJ}) + (-1\,836\text{ kJ}) = -802\text{ kJ}$$

We can now write the reaction as:

$$CH_4 + 2\,O_2 \rightarrow CO_2 + 2\,H_2O + 802\text{ kJ}$$

This agrees with the heat of reaction that we would calculate from enthalpy of formation data:

Compound	$\Delta H_f^\circ \left(\frac{\text{kJ}}{\text{mol}}\right)$
$CH_4(g)$	−74.8
$O_2(g)$	0
$CO_2(g)$	−393.5
$H_2O(g)$	−241.8

CH_4	+	$2\,O_2$	→	CO_2	+	$2\,H_2O$
$+74.8\frac{\text{kJ}}{\text{mol}}$		$2(0\frac{\text{kJ}}{\text{mol}})$		$-393.5\frac{\text{kJ}}{\text{mol}}$		$2(-241.8\frac{\text{kJ}}{\text{mol}})$
+74.8 kJ		0 kJ		−393.5 kJ		−483.6 kJ

$$74.8\text{ kJ} + 0 + (-393.5\text{ kJ}) + (-483.6\text{ kJ}) = -802.3\text{ kJ}$$

Note that adding the bond dissociation energies for a compound does not give the compound's enthalpy of formation. As an example, recall that the heat of formation of O_2 is zero, but it takes $494\frac{\text{kJ}}{\text{mol}}$ of heat energy to break an O=O double bond.

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Limitations of Using Bond Energy to Calculate Heat of Reaction

The above example with methane is one of the few instances where bond energies and heats of formation give the same values. This is often not the case. For example, if you calculate the heat of reaction for the combustion of acetylene:

$$2\ H{-}C{\equiv}C{-}H + 5\ O_2 \rightarrow 4\ CO_2 + 2\ H_2O + \text{heat}$$

you would get −2 511 kJ using heat of formation data, but −4 914 kJ using bond energies.

Enthalpies of formation are well-defined and precise, meaning that different people could measure them and expect to get the same answer. Average bond enthalpies, however, can vary widely depending on which molecules were used to gather the data. (In fact, the numbers may vary significantly from one published table to another.)

For example, there are many different molecules with C–H bonds. The bond energy of a C–H bond in CH_4 is very different from the bond energy of a C–H bond in acetylene.

The bond energies found in the bond energy tables for the bonds involved in the combustion of methane are based on:

Bond	C−H	C=O	O=O	O−H
Energy $\left(\frac{\text{kJ}}{\text{mol}}\right)$	411	799	494	459
Based on	CH_4	CO_2	O_2	H_2O

Needless to say, the basis for each of these bond energies is exactly the same as the bonds broken or formed in the combustion of methane. It is therefore not surprising that using bond energies gives the same result. However, it takes much more energy to break the C−H bond in acetylene, which is part of the reason that using bond energies does not give the correct answer for acetylene.

Because average bond enthalpies are much less accurate than enthalpies of formation, calculating heat of reaction from bond energies should only be used for a quick estimation, or as a last resort when heat of formation data are not available.

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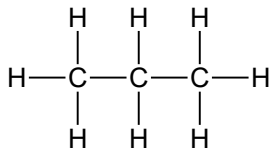
Homework Problem

1. Propane (C_3H_8) has the following structure:



Using the bond energy data from this chapter or on page 518 of your Chemistry reference tables, compute the heat of reaction for the complete combustion of propane:

$$C_3H_8 + 5\ O_2 \rightarrow 3\ CO_2 + 4\ H_2O + \text{heat}$$

Answer: −2 016 kJ (Note: calculating from ΔH_f^o values gives 2 044 kJ)

Use this space for summary and/or additional notes: