Bond energy and ΔH_{rxn}

Energy is said to be "stored" in chemical bonds. Think of it this way: when two atoms come together and form a bond, their potential energies are lowered – that is, they are more stable when bonded together than they were before they were bonded. That means it takes energy to pull the atoms back apart, or to "break" the bond. This amount of energy is referred to as the bond dissociation energy, and can be used to compare the relative strength of different bonds – the stronger the bond, the more energy it would take to break the bond. The bond dissociation energy is essentially the enthalpy change (ΔH) for breaking the bond. The bond dissociation energy is similar for similar types of bonds. For example, breaking the O-H bond in water takes a similar amount of energy as breaking the O-H bond in an alcohol. After extensive laboratory investigations, the amount of energy to break the O-H bonds in various different compounds has been determined, and an average value for the energy of a "typical" O-H bond has been established, as well as that of many other common covalent bonds, as can be seen in the table below.

Average Bond Dissociation Energies

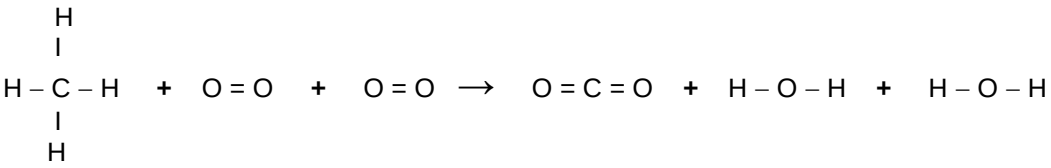
Single Bonds (kJ/mol)									
	H	**C**	**N**	**O**	**S**	**F**	**Cl**	**Br**	**I**
H	432								
C	411	346							
N	386	305	167						
O	459	358	201	142					
S	363	272	-	364	226				
F	565	485	283	190	284	155			
Cl	428	327	313	218	255	249	240		
Br	362	285	-	201	217	249	216	190	
I	295	213	-	201	-	278	208	175	149
Multiple Bonds									
C=C	602		**C=N**	615		**C=O**	799		
C≡C	835		**C≡N**	887		**C≡O**	1072		
N=N	418		**N=O**	607		**S=O**	532	**(SO2)**	
N≡N	942		**O=O**	494					

In the course of a chemical reaction, many bonds are broken as the reactants become the products – and new bonds are formed as well. Although energy must *go into* the system to break the bonds in the reactants, when the new bonds in the products are formed the potential energy of the atoms in the newly formed products decreases, and energy is *released*. One way to approximate the ΔH for a reaction (in a process similar to calculating ΔH using heats of formation) is to calculate the energy that would be necessary to break all of the bonds in the reactant molecules, and compare that to the energy released when the new bonds in the products are formed.

ΔH = (sum of the bond energies for broken bonds) + (sum of bond energies for bonds formed)

Note : Thermochemical data is usually a more accurate way to determine ΔH for a reaction, but bond energies may be considered to calculate an approximate value. In addition, the bond energies are useful for considering which bonds are "stronger" and which are relatively "weaker". In general, if, through the course of a reaction, weak bonds are broken and strong bonds are formed, the reaction will be exothermic.

Consider the reaction: **$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$**



To break all of the bonds in the reactant molecules would **require** breaking 4 C-H bonds and 2 O=O bonds:

(**4** x **411kJ**) + (**2** x **494kJ**) = **2632kJ**

To form the products, 2 C=O bonds and 4 H-O bonds are formed, **releasing**:

(**2** x **799kJ**) + (**4** x **459kJ**) = **-3434kJ** *note: negative number, as this energy is released*

This means that although 2632kJ of energy must *go into* the reactants to break their bonds, 3434kJ of energy is *released* when the new bonds that exist in the products are formed.

Therefore, **ΔH_{rxn}** = **2632kJ** + **-3434kJ** = **-802kJ**, and the reaction is *exothermic*, as one would expect from a combustion.

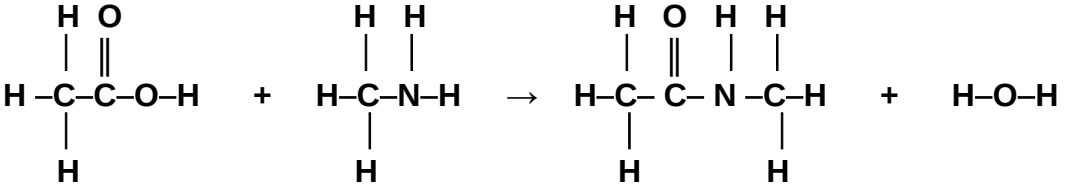
Draw structures for the following formulas, and calculate the ΔH for the reactions indicated:

$SO_2 + 3\ F_2 \rightarrow SF_6 + O_2$

ΔH_{rxn} =

$2\ CH_4 + Cl_2 \rightarrow 2\ CH_3Cl + H_2$

ΔH_{rxn} =



{ $CH_3COOH + CH_3NH_2 \rightarrow CH_3CONHCH_3 + H_2O$ }

ΔH_{rxn} =