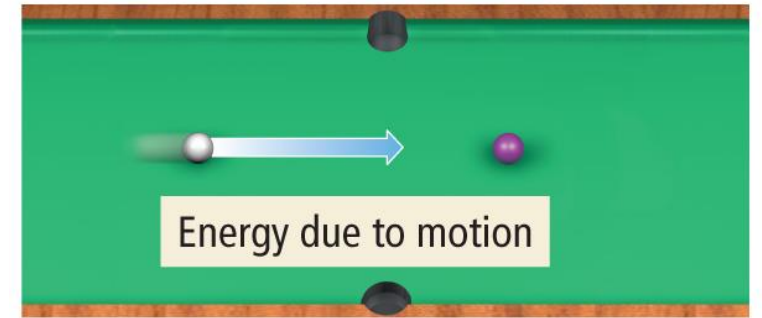


THERMOCHEMISTRY

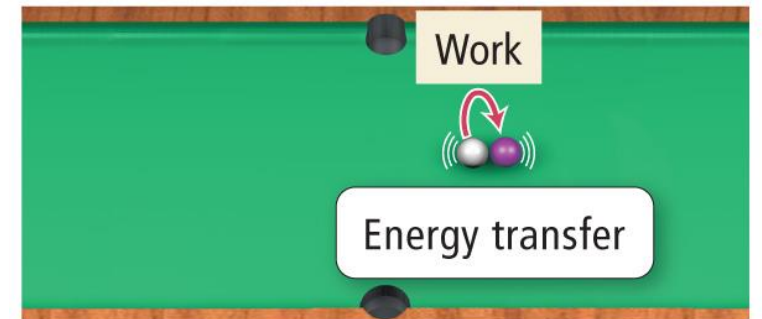
Heat of Formation

Classification of Energy

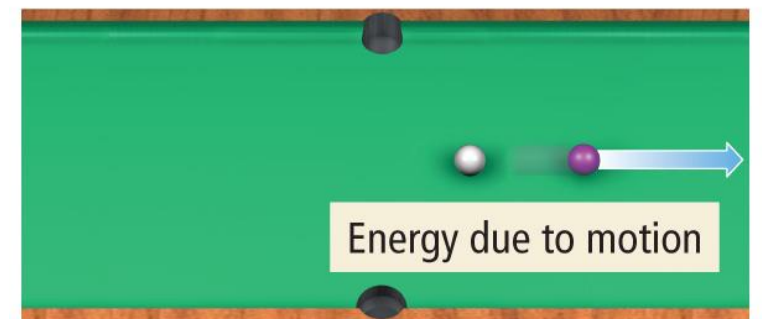
- **Kinetic energy** is energy of motion or energy that is being transferred.
- **Thermal energy** is the energy associated with temperature.
 - Thermal energy is a form of kinetic energy.



(a)



(b)



(c)

Formation Reactions

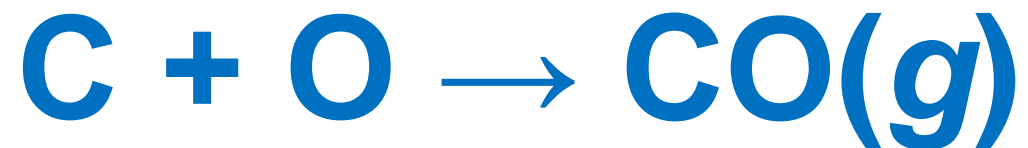
Reactions of elements in their “standard state” to form 1 mole of a pure compound.

- **Standard State** of an element - find the form in Appendix IIB that has $\Delta H_f^\circ = 0$.
- Coefficients of the reactants may be fractions!
 - *Because* the definition requires 1 mole of compound be made.

Writing Formation Reactions

Write the formation reaction for CO (g)

- The formation reaction is the reaction between the elements in the compound, which are C and O.



Writing Formation Reactions

Write the formation reaction for CO (g)

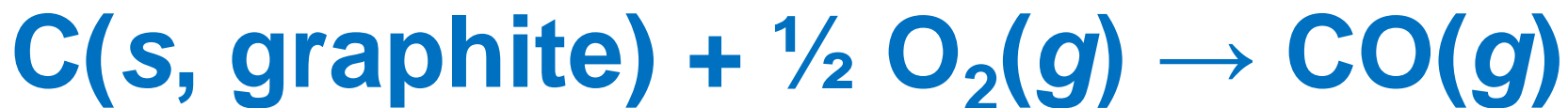
- The elements must be in their standard state.
 - There are several forms of solid C, but the one with $\Delta H_f^\circ = 0$ is graphite.
 - Oxygen's standard state is the diatomic gas.



Writing Formation Reactions

Write the formation reaction for CO (g)

- The equation must be balanced, but the coefficient of the product compound must be 1.
 - Use whatever coefficient in front of the reactants is necessary to make the atoms on both sides equal without changing the product coefficient.



Calculating Standard Enthalpy Change For a Rxn

Any reaction can be written as the sum of formation reactions (or the reverse of formation reactions) for the reactants and products.

The ΔH° for the reaction is then the sum of the ΔH_f° for the component reactions.

$$\Delta H^\circ = \Sigma n \Delta H_f^\circ(\textit{products}) - \Sigma n \Delta H_f^\circ(\textit{reactants})$$

- Σ means sum.
- n is the coefficient of the reaction.

Calculating Heat of Rxn from Heats of Formation

Calculate ΔH for the combustion of methane, CH_4

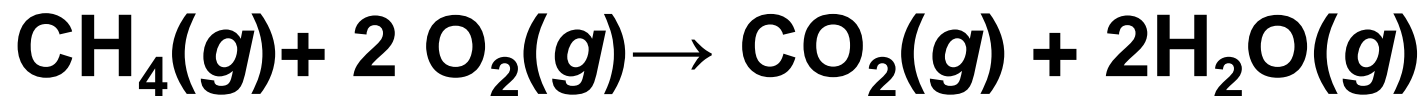


$$\Delta H^\circ = \sum n\Delta H_f^\circ(\text{products}) - \sum n\Delta H_f^\circ(\text{reactants})$$

<u>Substance</u>	<u>ΔH_f</u> (kJ)
CH_4	-74.80
O_2	0
CO_2	-393.50
H_2O	-285.83

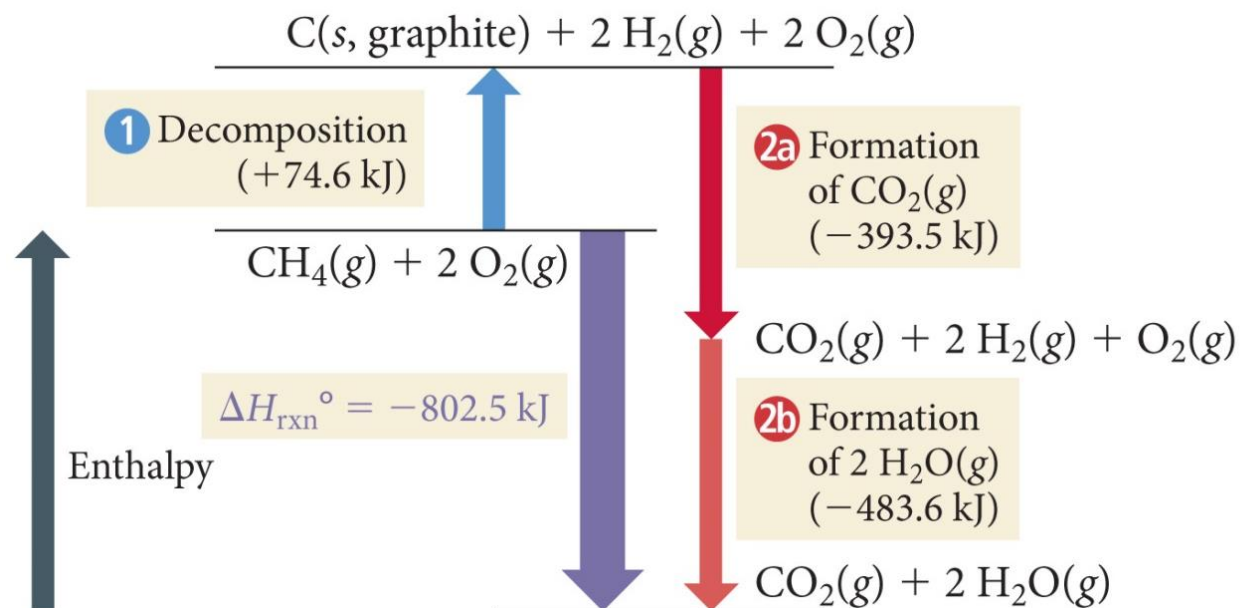
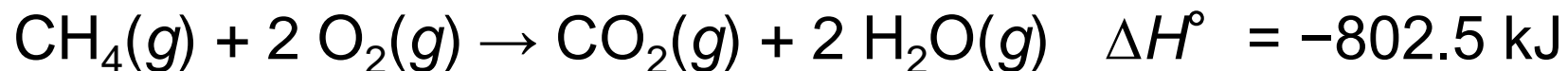
$$\Delta H_{\text{rxn}} = [-393.50\text{kJ} + 2(-285.83\text{kJ})] - [-74.80\text{kJ}]$$

$$\Delta H_{\text{rxn}} = \mathbf{-890.36 \text{ kJ}}$$



$$\Delta H^\circ = [\Delta H_f^\circ(\text{CO}_2) + 2 \cdot \Delta H_f^\circ(\text{H}_2\text{O})] - [\Delta H_f^\circ(\text{CH}_4) + 2 \cdot \Delta H_f^\circ(\text{O}_2)]$$

$$\Delta H^\circ = [((-393.5 \text{ kJ}) + 2(-241.8 \text{ kJ}) - ((-74.6 \text{ kJ}) + 2(0 \text{ kJ})))] = -802.5 \text{ kJ}$$

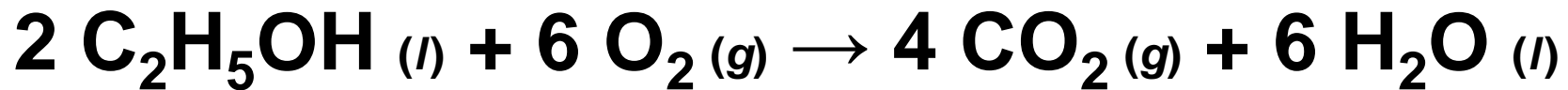


Notice anything about the #'s on last two slides?

- The numbers can vary slightly based on the appendix used. Always use numbers given to you in the problem, otherwise look them up and don't stress if they don't exactly match someone else's
- One H₂O was gas, one was liquid! Phase matters!
Be careful!

Ethanol is used as an additive in many fuels today.

What is $\Delta H^\circ_{\text{rxn}}$ (kJ) for the combustion of ethanol?

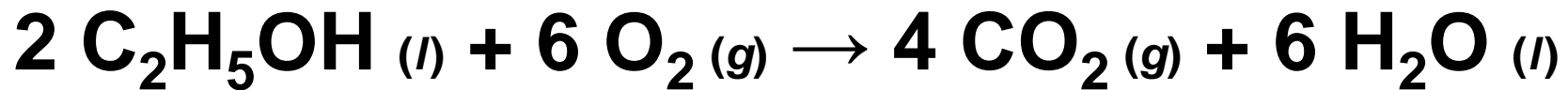


Formula	ΔH°_f
$\text{C}_2\text{H}_5\text{OH} (l)$	-277.6
$\text{CO}_2 (g)$	-393.5
$\text{H}_2\text{O} (g)$	-241.8
$\text{H}_2\text{O} (l)$	-285.8

- A** - 401.7
- B** + 401.7
- C** - 2469
- D** + 2734
- E** - 2734

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A - 401.7

B + 401.7

C - 2469

D + 2734

E - 2734

$$\Delta H^\circ_{\text{rxn}} = \text{Products} - \text{Reactants}$$

$$[4(-393.5) + 6(-285.8)] - [2(-277.6) + 6(0)]$$

$$= \mathbf{-2734 \text{ kJ/mol}}$$

Bond Energy

Slightly different than Enthalpy of Formation.

Values will be given to you in a chart

Two Ways to think about it:

$$\Sigma H_{(\text{Bonds Broken})} - \Sigma H_{(\text{Bonds Formed})}$$

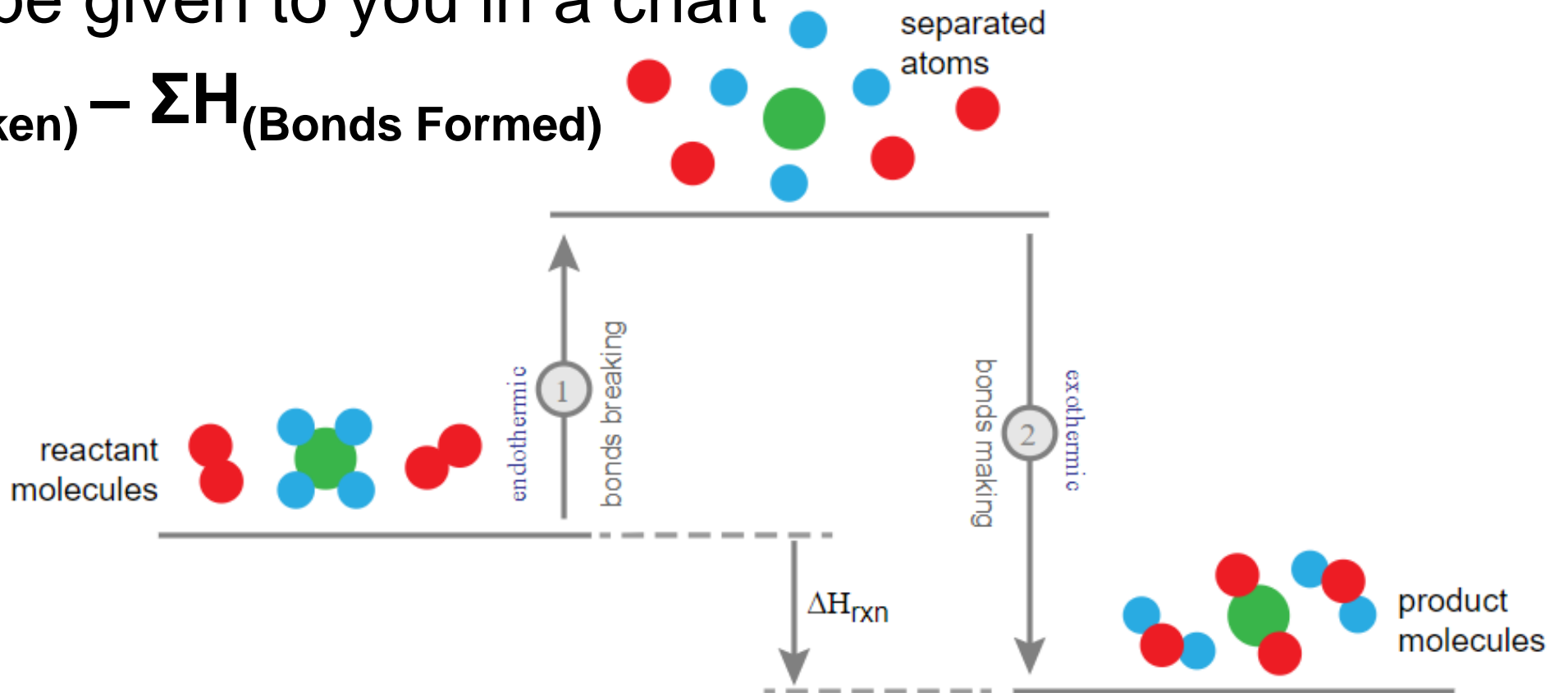
The reason this way can be tricky, is because almost everything in chemistry is thought of as “products minus reactants” and this is one of the very few times it is backwards! A lot of mistakes happen here.

Bond Energy

Slightly different than Enthalpy of Formation.

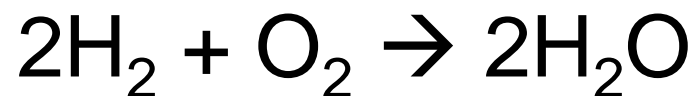
Values will be given to you in a chart

$$\Sigma H_{(\text{Bonds Broken})} - \Sigma H_{(\text{Bonds Formed})}$$



1st Way to Think About It

$$\Sigma H_{(\text{Bonds Broken})} - \Sigma H_{(\text{Bonds Formed})}$$



You have to break: 2 H-H bond and 1 O=O bond

You have to form: 4 H-O bonds

$$[2(436) + (498)] - [4(463)] = - 482 \text{ kJ/mol (exo)}$$

Can be tricky though because almost everything in chemistry is thought of as “Products minus Reactants” and this is one of the few times it is the opposite!

Single Bond Energies (kJ/mol of bonds)

	H	C	N	O	S	F	Cl	Br	I
H	436								
C	413	346							
N	391	305	163						
O	463	358	201	146					
S	347	272	—	—	226				
F	565	485	283	190	284	155			
Cl	432	339	192	218	255	253	242		
Br	366	285	—	201	217	249	216	193	
I	299	213	—	201	—	278	208	175	151

Multiple Bond Energies (kJ/mol of 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		
N≡N	945	O=O	498		

2nd Way to Think About It

Action	Algebraic Sign	How to Remember
Break a Bond	+	Takes to Break
Form a Bond	-	Free to Form

Nice thing about this method is that it doesn't matter if you do broken or formed first – see?

You have to form: 4 H-O bonds

You have to break: 2 H-H bond and 1 O=O bond

$$4(-463) + 2(436) + (498) = \mathbf{-482 \text{ kJ/mol}} \text{ (exo)}$$

Same answer as before! Doesn't matter which way you do it as long as you are explicit with what you are doing. Either write the equation from the 1st way, or something about takes to break, free to form for the 2nd way.

Single Bond Energies (kJ/mol of bonds)

	H	C	N	O	S	F	Cl	Br	I
H	436								
C	413	346							
N	391	305	163						
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