N4 - THERMOCHEMISTRY

Heat of Formation

Link to YouTube Presentation: https://youtu.be/w7LzmmIrF-8

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Heat of Formation

Target: I can use Heat of Formation data or Bond Energy data to calculate the overall enthalpy required to form a product.

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 that has $\Delta H_f°$ = 0.

- Coefficients of the reactants may be fractions!
- *Because* definition requires 1 mole of compound be made

Writing Formation Reactions

Write the formation reaction for CO (g)

- Start with the reaction between the **elements** in the compound, which are C and O.

$$C + O \rightarrow CO(g)$$

Writing Formation Reactions

Write the formation reaction for CO (g)

- Then make sure elements are in their **standard state**.
  - There are several forms of solid C,
    but the one with $\Delta H_f°$ = 0 is graphite.
  - Oxygen's standard state is the diatomic gas.

$$\mathrm{C(s,\ graphite)} + \mathrm{O_2}(g) \rightarrow \mathrm{CO}(g)$$

Writing Formation Reactions

Write the formation reaction for CO (g)

- Then balance the equation 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.

$$\mathbf{1\ C(\mathit{s}, graphite) + \tfrac{1}{2}\ O_2(\mathit{g}) \rightarrow 1\ CO(\mathit{g})}$$

Why does product have to be ONE mole?
Because that is how they chose to define it!

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 $\Delta H°$ for the reaction is then the sum of the $\Delta H_f°$ for the component reactions.

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

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

Calculating Heat of Rxn from Heats of Formation

Practice #1 - Calculate ΔH for the combustion of methane, CH_4

$$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l)$$

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

Substance	**ΔH_f (kJ)**
CH_4	-74.80
O_2	0
CO_2	-393.50
H_2O	-285.83

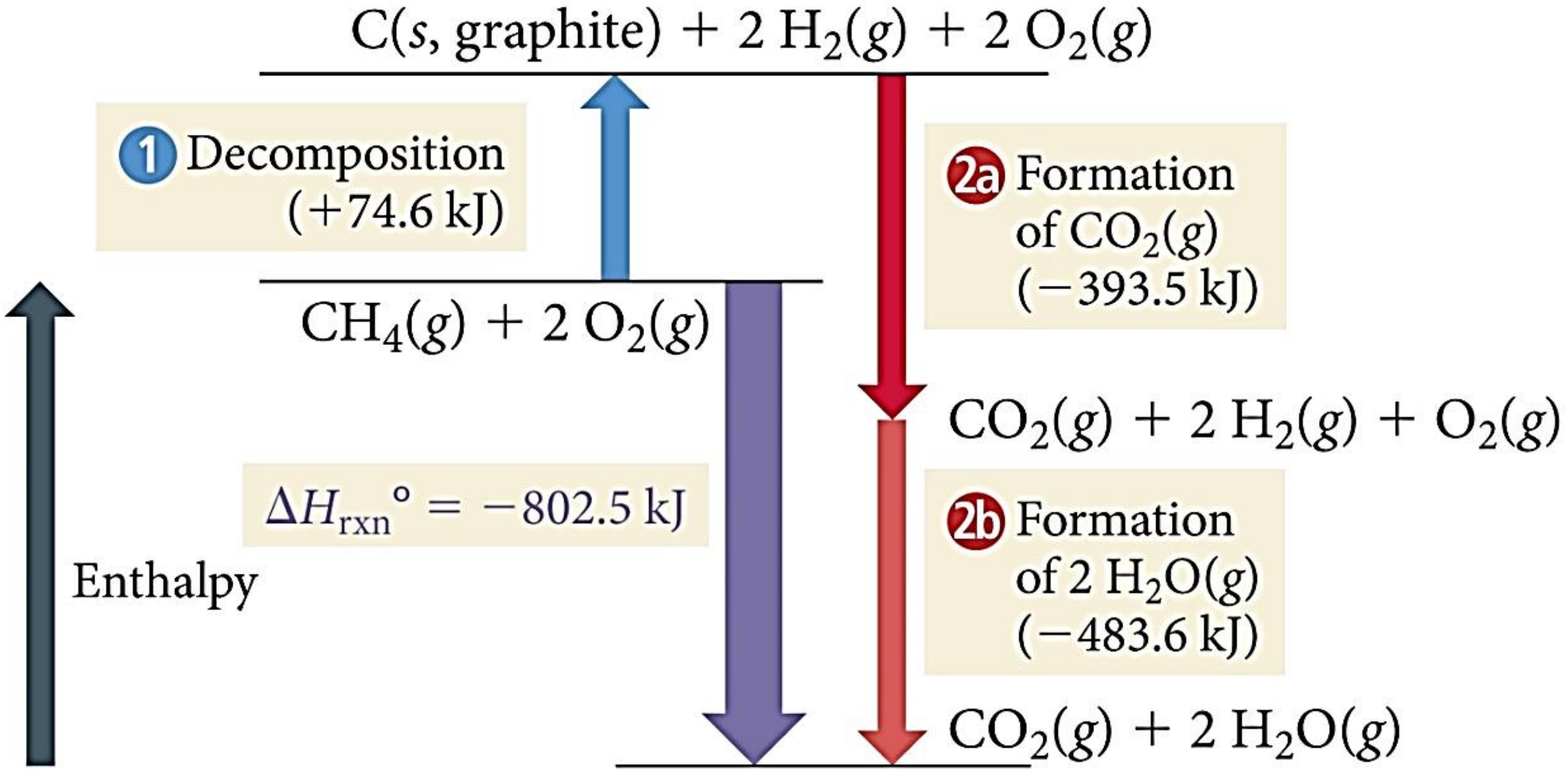
$$\Delta H_{rxn} = [-393.50kJ + 2(-285.83kJ)] - [-74.80kJ + 2(0kJ)]$$

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

Slightly different this time…$CH_4(g)$+ 2 $O_2(g)$→ $CO_2(g)$ + 2$H_2O(g)$

$$\Delta H^{\circ} = \left[\Delta H_f^{\circ}(CO_2) + 2 \cdot \Delta H_f^{\circ}(H_2O)\right] - \left[\Delta H_f^{\circ}(CH_4) + 2 \cdot \Delta H_f^{\circ}(O_2)\right]$$

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



$C(s, \text{graphite}) + 2\ H_2(g) + 2\ O_2(g)$

① Decomposition (+74.6 kJ)

2a Formation of $CO_2(g)$ (−393.5 kJ)

$CH_4(g) + 2\ O_2(g)$

$CO_2(g) + 2\ H_2(g) + O_2(g)$

$\Delta H_{rxn}° = -802.5$ kJ

Enthalpy

2b Formation of 2 $H_2O(g)$ (−483.6 kJ)

$CO_2(g) + 2\ H_2O(g)$

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 H_2O was gas, one was liquid!

Phase matters!
Be careful!

Practice #2 - Ethanol is used as an additive in many fuels today. What is ΔH^{o}_{rxn} (kJ) for the combustion of ethanol?

$$2\ C_2H_5OH_{(l)} + 6\ O_{2\,(g)} \longrightarrow 4\ CO_{2\,(g)} + 6\ H_2O_{(l)}$$

Formula	ΔH^{o}_{f}
C_2H_5OH (*l*)	–277.6
CO_2 (*g*)	–393.5
H_2O (*g*)	–241.8
H_2O (*l*)	–285.8

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

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

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

= **-2734 kJ/mol$_{rxn}$**

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.**

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Slightly different than Enthalpy of Formation.

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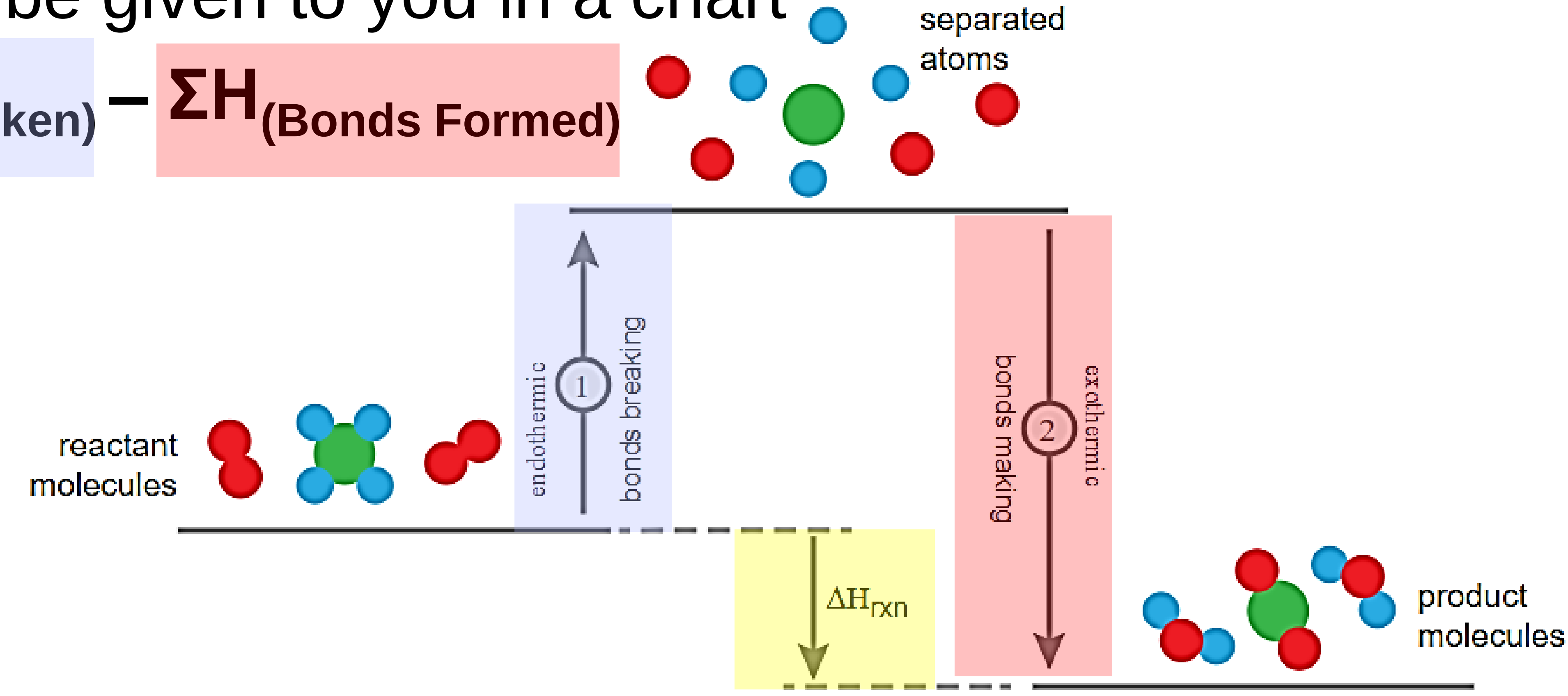
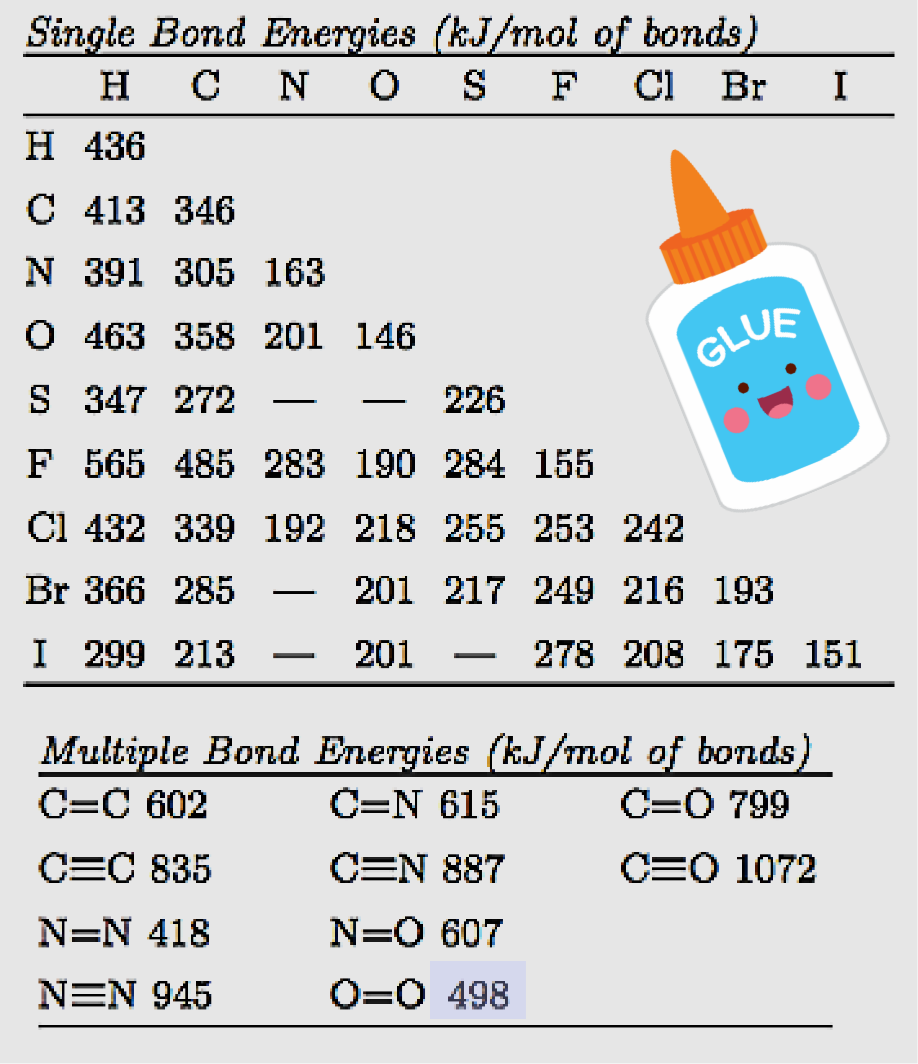


Practice #3

What is the enthalpy of formation for the equation below, using the table of bond energies provided.

$2H_2 + O_2 \rightarrow 2H_2O$



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	

1st Way to Think About It

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

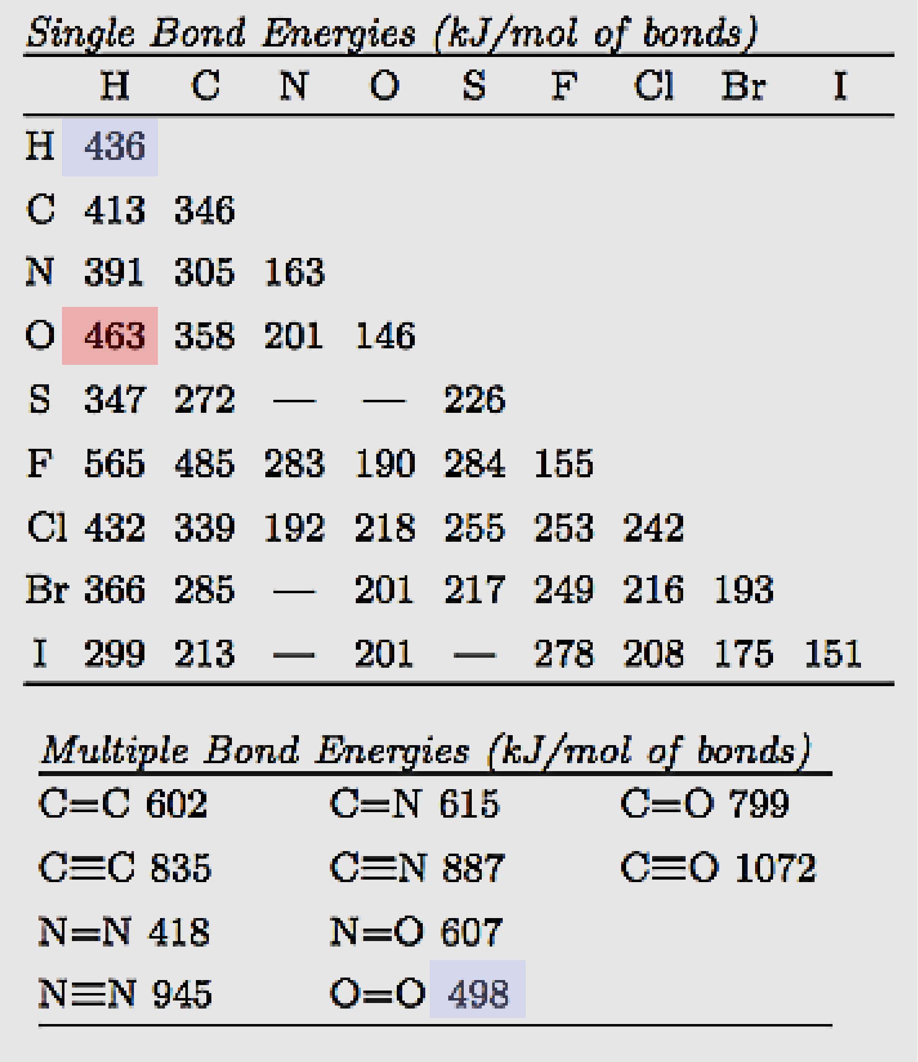
$2H_2 + O_2 \rightarrow 2H_2O$

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 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!



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BETTER Way…

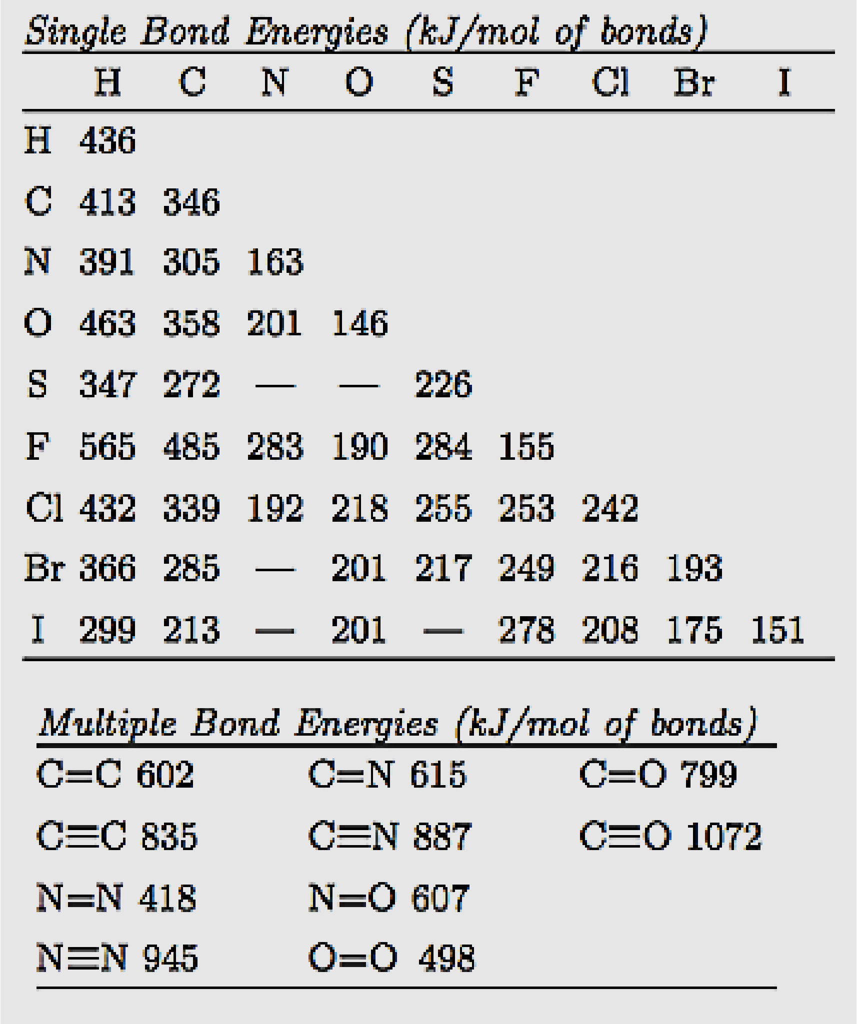
Action	Algebraic Sign	How to Remember
Break a Bond	+	Takes to Break
Form a Bond	-	Free to Form

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

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

You have to form: 4 H-O bonds

2(436) + (498) + 4(- 463)= **- 482 kJ/mol** (exo)



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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.

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