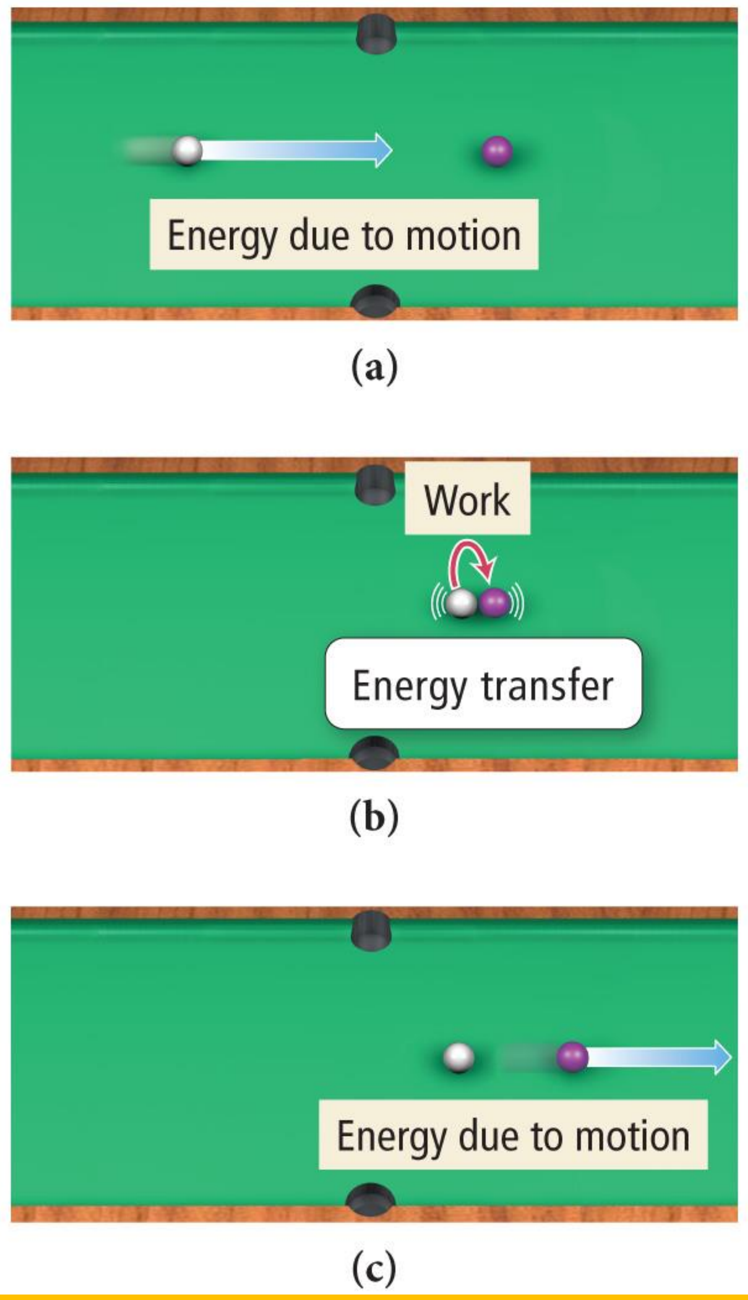
# N3 - THERMOCHEMISTRY

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.



# 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 $\Delta H_f° = 0$.
- 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.

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

# 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 $\Delta H_f°$ = 0 is graphite.
  - Oxygen's standard state is the diatomic gas.

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

# 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.

$$C(s, \text{graphite}) + \frac{1}{2} O_2(g) \rightarrow CO(g)$$

# 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.

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

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

# Calculating Heat of Rxn from Heats of Formation

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** | **$\Delta H_f$ (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]

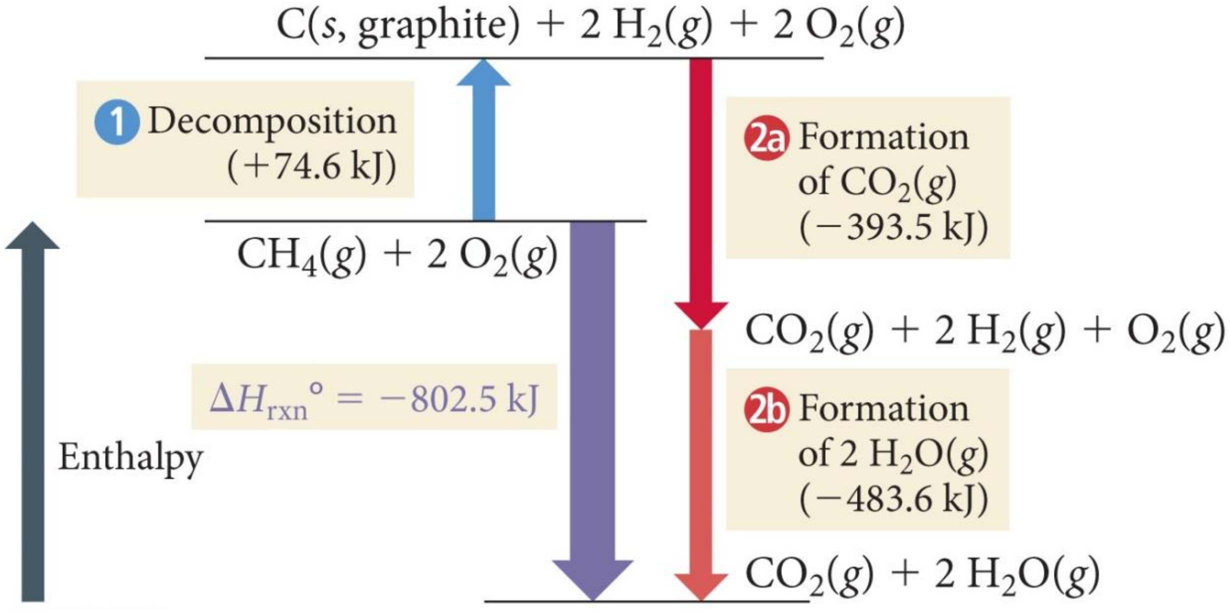
**$\Delta H_{rxn}$ = -890.36 kJ**

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

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

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

$$CH_4(g) + 2\,O_2(g) \rightarrow CO_2(g) + 2\,H_2O(g) \quad \Delta H^\circ = -802.5\text{ kJ}$$



# 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 $H_2O$ was gas, one was liquid! Phase matters! **Be careful!**

Ethanol is used as an additive in many fuels today.

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

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

| **Formula** | **$\Delta H^o_f$** |
|---|---|
| $C_2H_5OH$ (*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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E **- 2734**

$\Delta H^o_{rxn} =$ *Products – Reactants*

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

= **-2734 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.

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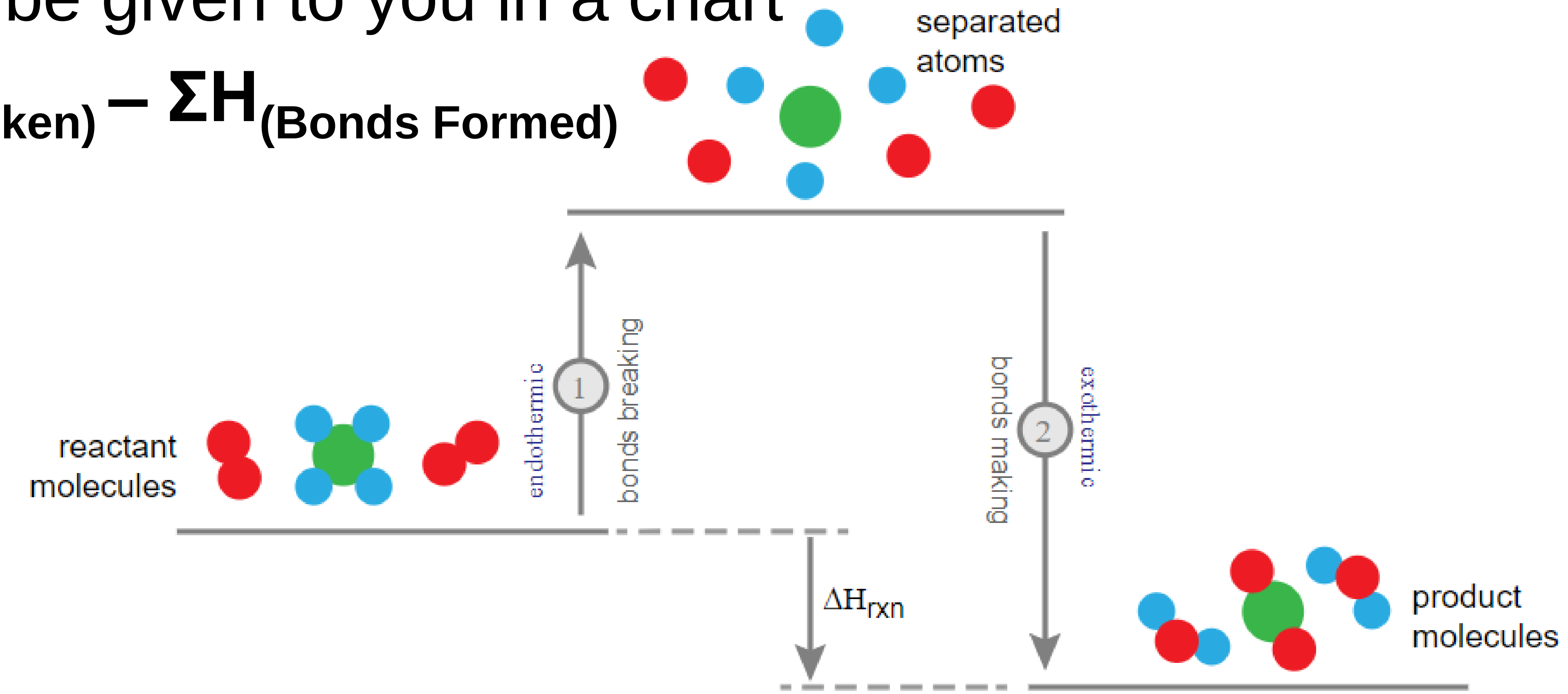

# $1^{st}$ Way to Think About It

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

$2H_2 + O_2 \rightarrow 2H_2O$

**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!

*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 | |

# $2^{nd}$ 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) = **- 482 kJ/mol** (exo)

*Single Bond Energies (kJ/mol of bonds)*

| | H | C | N | O | S | F | Cl | Br | I |
|---|---|---|---|---|---|---|---|---|---|
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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 $1^{st}$ way, or something about takes to break, free to form for the $2^{nd}$ way.