

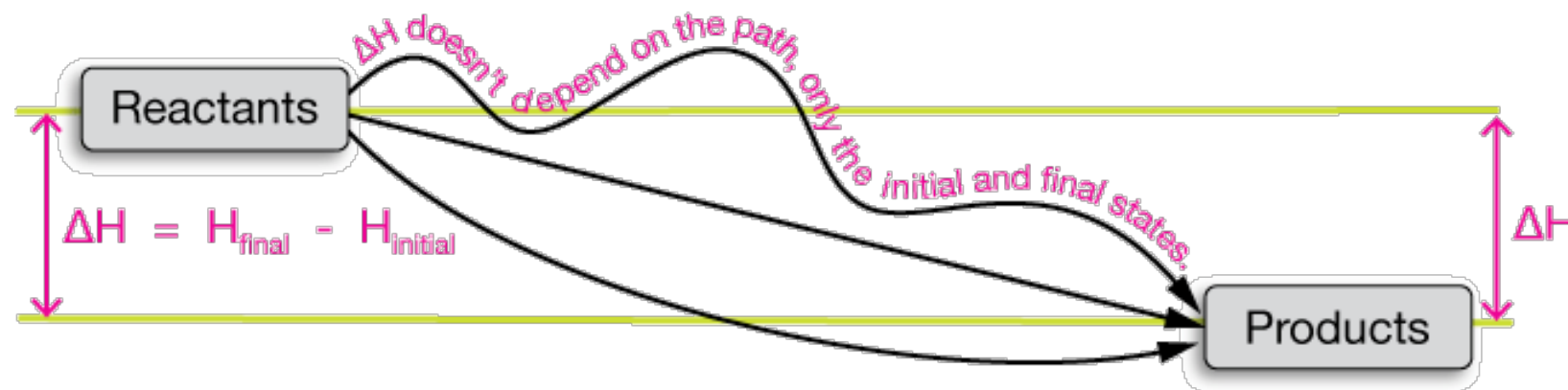
# Bond Enthalpies & Strengths

**DR. MIOY T. HUYNH**  
YALE UNIVERSITY  
CHEMISTRY 161  
FALL 2019

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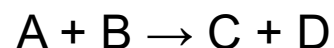
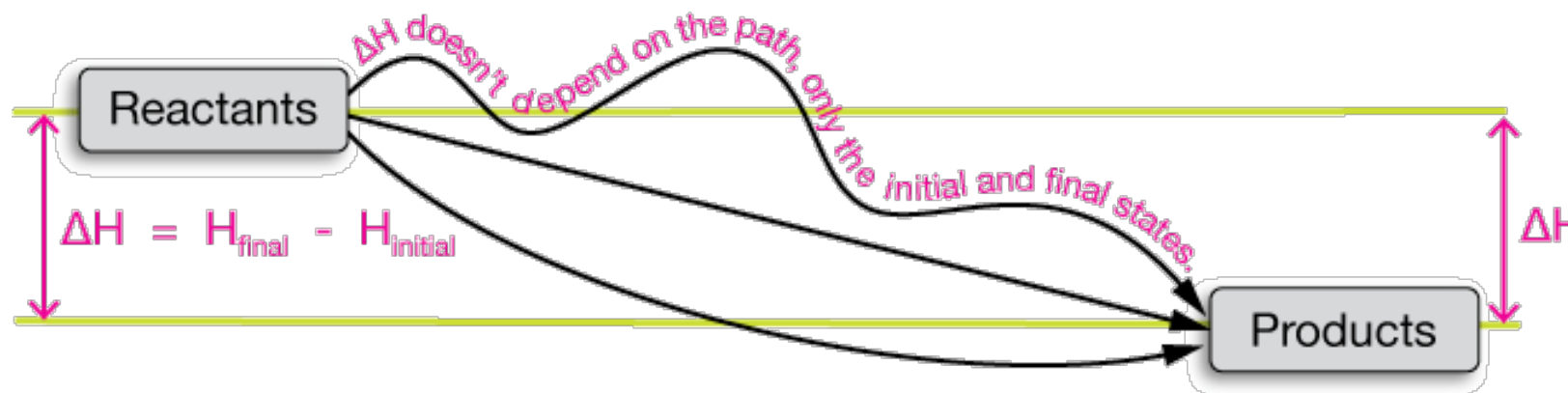
## Review: Heats of Reactions ( $\Delta H$ )

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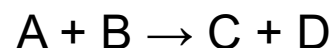
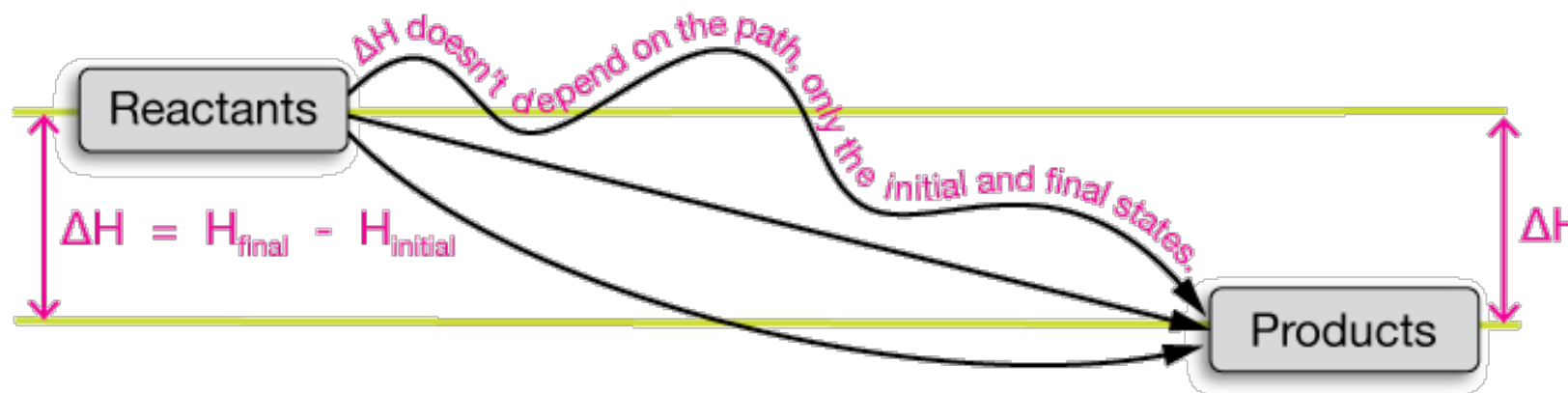


For a particular chemical reaction (above), we can use any of the following methods to calculate the  $\Delta H_{\text{rxn}}$ :

- Calorimetry: measure the heat absorbed ( $q_{\text{abs}}$ ) by surrounding water, where  $q_{\text{abs}} = -\Delta H_{\text{rxn}}$
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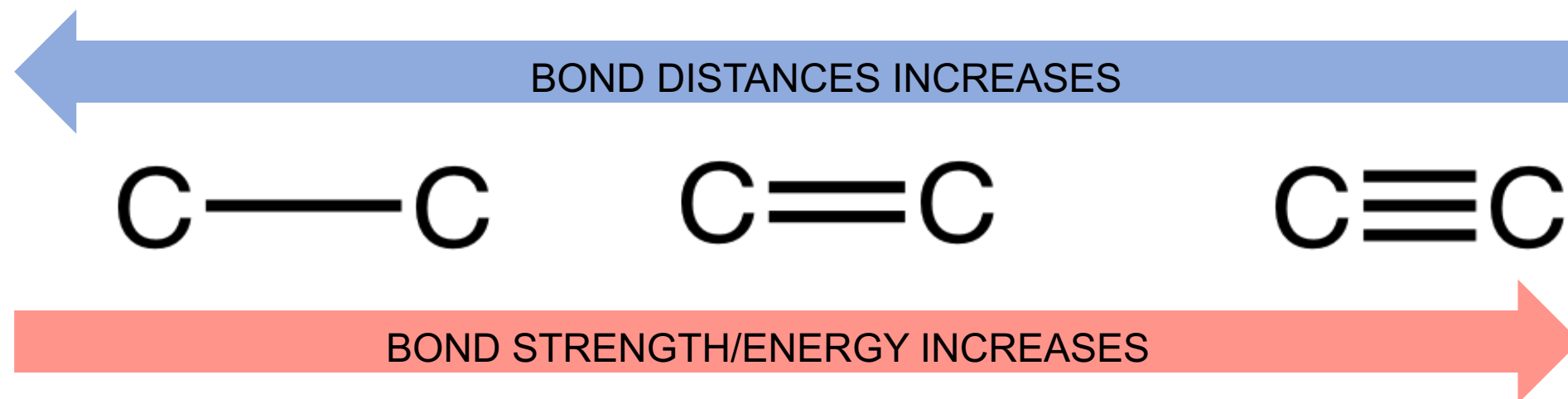


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- Apply Hess's Law on related chemical reactions with known  $\Delta H_{\text{rxn}}$
- Estimate using bond enthalpies ( $\Delta H$ ) for bonds broken and bonds formed during the reaction

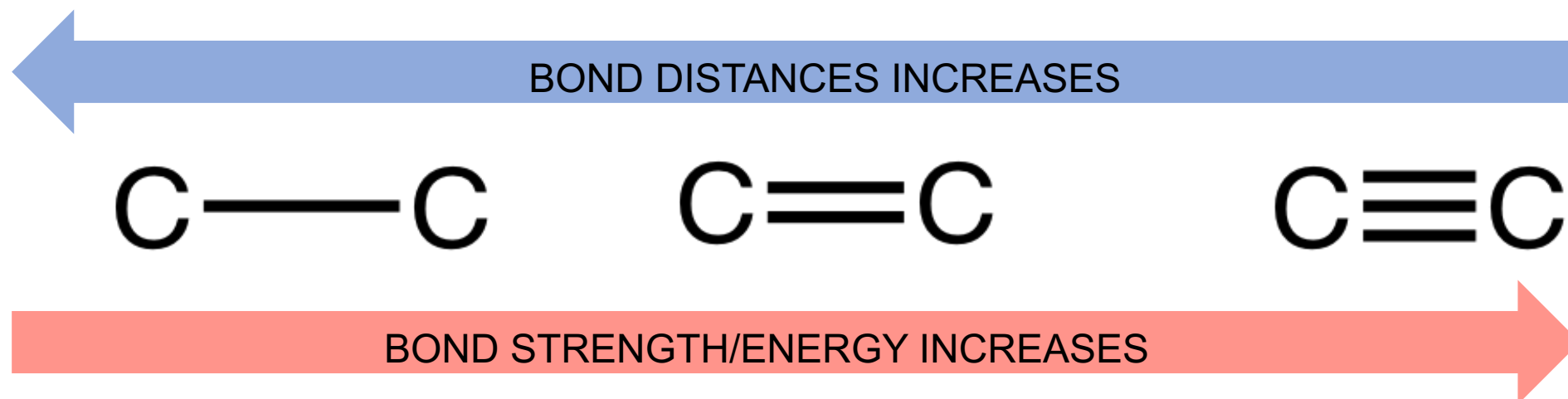
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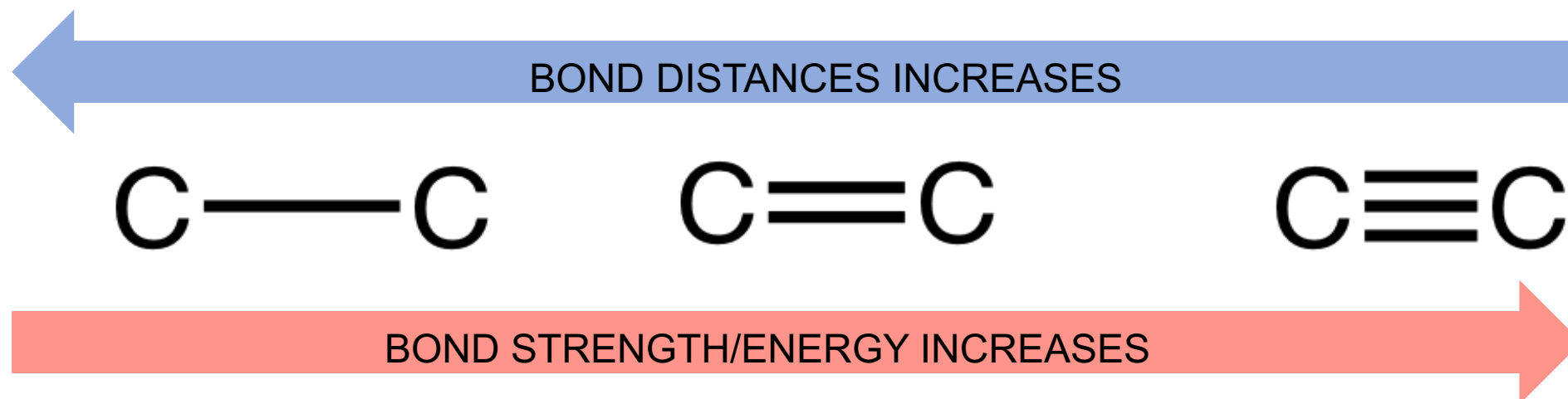


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$$\Delta H_{\text{rxn}} \approx \sum \Delta H(\text{bonds broken in reactants}) - \sum \Delta H(\text{bonds formed in products})$$

*By definition, all bond enthalpies are positive values.*

# Bond Enthalpies

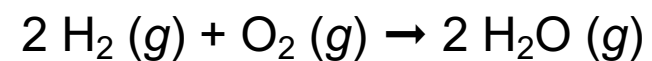
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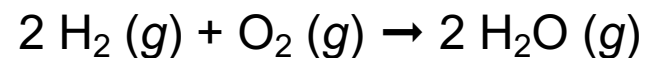
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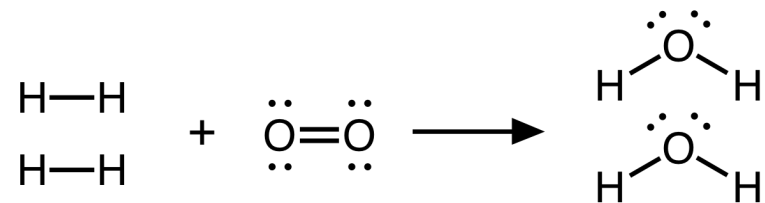
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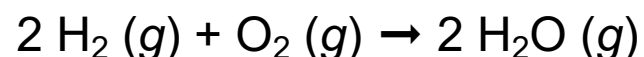
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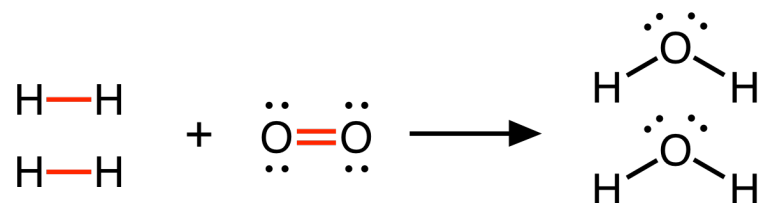
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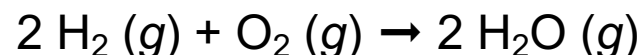
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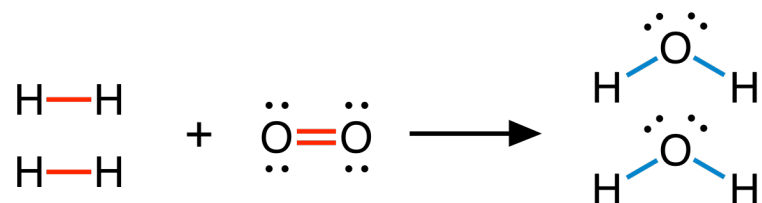
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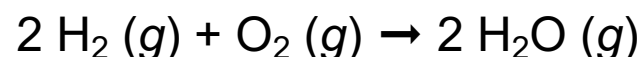
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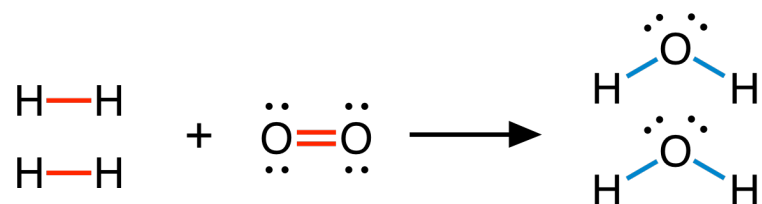
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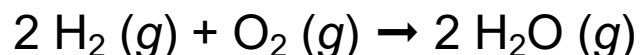
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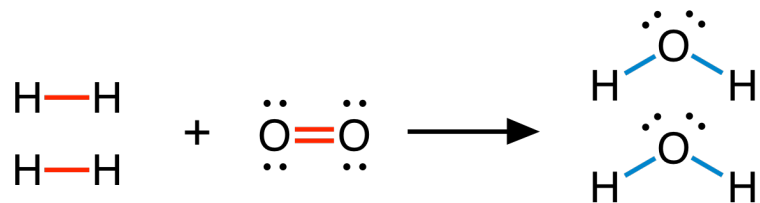
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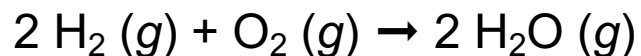
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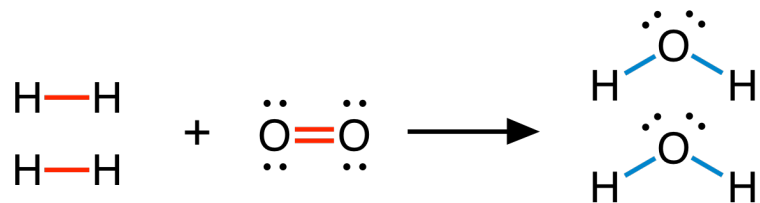
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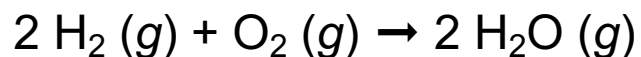
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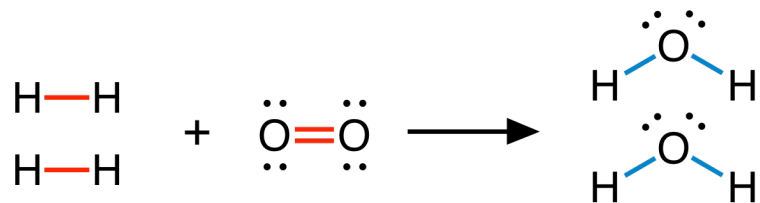
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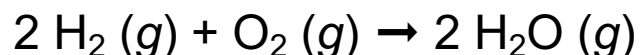
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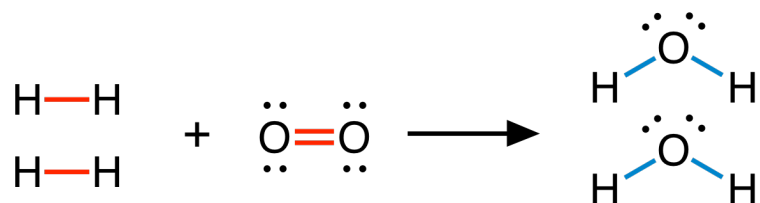
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As a double-check, the standard heat of formation of  $\text{H}_2\text{O} (g)$  is  $\Delta H_f^\circ = -241.8 \frac{\text{kJ}}{\text{mol}}$ .

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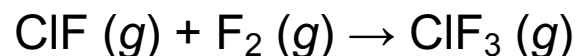
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<sup>a</sup>The bond energy of the C=O bond in  $\text{CO}_2$  is 799 kJ/mol.

**A more interesting example:**

## Previously, we used Hess's Law to find $\Delta H_{\text{rxn}}$

Let's say you want to calculate the heat of reaction for the following reaction:



You have access to the heats of reactions of some related reactions:

- |     |   |                                |
|-----|---|--------------------------------|
| (1) | $2\text{OF}_2 (g) \rightarrow \text{O}_2 (g) + 2\text{F}_2 (g)$                                   | $\Delta H = -49.4 \text{ kJ}$  |
| (2) | $2\text{ClF} (g) + \text{O}_2 (g) \rightarrow \text{Cl}_2\text{O} (g) + \text{OF}_2 (g)$          | $\Delta H = +205.6 \text{ kJ}$ |
| (3) | $\text{ClF}_3 (g) + \text{O}_2 (g) \rightarrow 1/2 \text{Cl}_2\text{O} (g) + 3/2 \text{OF}_2 (g)$ | $\Delta H = +266.7 \text{ kJ}$ |

Now sum up reactions (2), (1), and (3):

- |     |   |   |
|-----|---|---|
| (2) | $\text{ClF} (g) + \cancel{1/2 \text{O}_2 (g)} \rightarrow 1/2 \text{Cl}_2\text{O} (g) + \cancel{1/2 \text{OF}_2 (g)}$ | $\Delta H = 1/2 (+205.6 \text{ kJ})$        |
| (1) | $\text{F}_2 (g) + \cancel{1/2 \text{O}_2 (g)} \rightarrow \cancel{\text{OF}_2 (g)}$                                   | $\Delta H = 1/2 (+49.4 \text{ kJ})$         |
| (3) | $1/2 \text{Cl}_2\text{O} (g) + 3/2 \cancel{\text{OF}_2 (g)} \rightarrow \text{ClF}_3 (g) + \cancel{\text{O}_2 (g)}$   | $\Delta H = -266.7 \text{ kJ}$              |
|     | $\text{ClF} (g) + \text{F}_2 (g) \rightarrow \text{ClF}_3 (g)$  | $\Delta H_{\text{rxn}} = -139.2 \text{ kJ}$ |

**CAN WE USE BOND ENTHALPIES INSTEAD?**

## Example: $\text{ClF}_3 (g)$

In order to estimate the heat of a reaction ( $\Delta H_{\text{rxn}}$ ), you need to:

- Balance the chemical equation

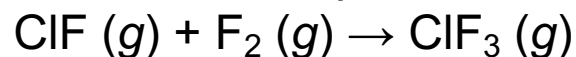


TABLE 8.3 Selected Average Covalent Bond Lengths and Bond Energies

Bond	Bond Length (pm)	Bond Energy (kJ/mol)	Bond	Bond Length (pm)	Bond Energy (kJ/mol)
C—C	154	348	N≡O	106	678
C=C	134	614	O—O	148	146
C≡C	120	839	O=O	121	495
C—N	147	293	O—H	96	463
C=N	127	615	S—O	151	265
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C—O	143	358	S—S	204	266
C=O	123	743 <sup>a</sup>	S—H	134	347
C≡O	113	1072	H—H	75	436
C—H	110	413	H—F	92	567
C—F	133	485	H—Cl	127	431
C—Cl	177	328	H—Br	141	366
N—H	104	388	H—I	161	299
N—N	147	163	F—F	143	155
N=N	124	418	Cl—Cl	200	243
N≡N	110	941	Br—Br	228	193
N—O	136	201	I—I	266	151
N=O	122	607	Cl—F		256

<sup>a</sup>The bond energy of the C=O bond in  $\text{CO}_2$  is 799 kJ/mol.

## Example: $\text{ClF}_3 (g)$

In order to estimate the heat of a reaction ( $\Delta H_{\text{rxn}}$ ), you need to:

- Balance the chemical equation  

$$\text{ClF} (g) + \text{F}_2 (g) \rightarrow \text{ClF}_3 (g)$$
- Draw out the Lewis structures of reactants and products

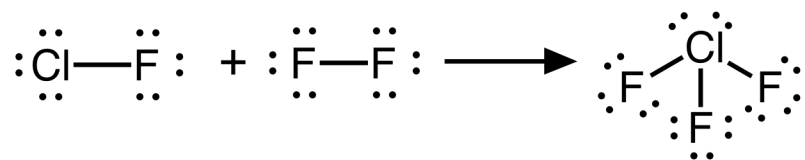


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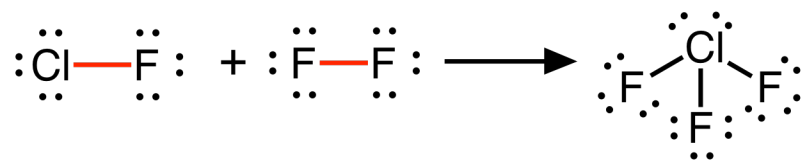
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In order to estimate the heat of a reaction ( $\Delta H_{\text{rxn}}$ ), you need to:

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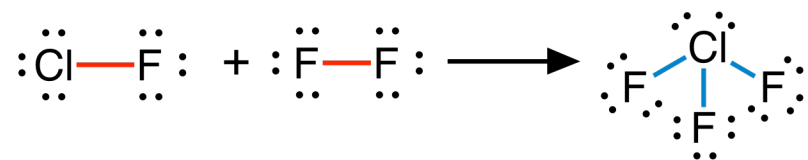
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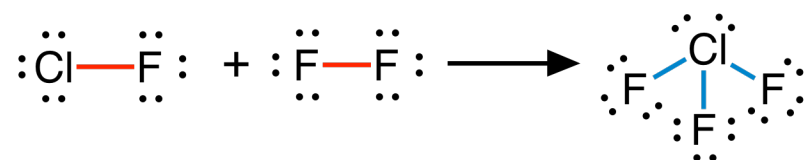
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Q: Did we really need to break the **Cl-F bond** in the reactants?

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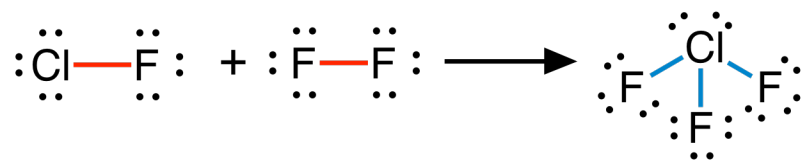


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**Q:** Did we really need to break the **Cl-F bond** in the reactants?  
**A:** No, we just need to form two more **Cl-F bonds** in the products.

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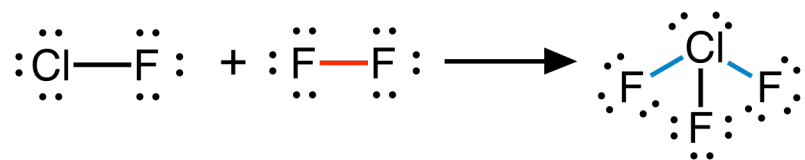
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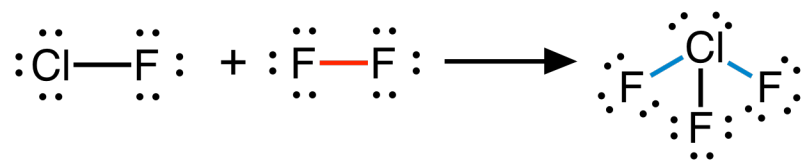
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**Q:** Did we really need to break the **Cl–F bond** in the reactants?

**A:** No, we just need to form two more **Cl–F bonds** in the products.

$$\begin{aligned} \Delta H_{\text{rxn}} &\approx \sum \Delta H \left( \begin{array}{l} \text{bonds broken} \\ \text{in reactants} \end{array} \right) - \sum \Delta H \left( \begin{array}{l} \text{bonds formed} \\ \text{in products} \end{array} \right) \\ &= (1 \text{ mol} \times \Delta H_{\text{F-F}}) - (2 \text{ mol} \times \Delta H_{\text{Cl-F}}) \\ &= \left( 1 \text{ mol} \times 155 \frac{\text{kJ}}{\text{mol}} \right) - \left( 2 \text{ mol} \times 256 \frac{\text{kJ}}{\text{mol}} \right) \\ \Delta H_{\text{rxn}} &\approx -357 \text{ kJ} \end{aligned}$$

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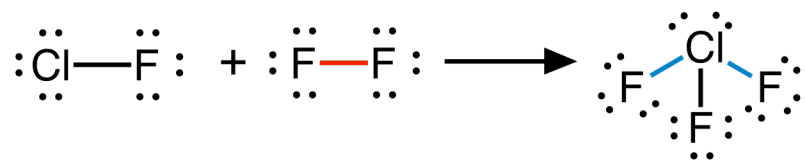
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**Q:** Did we really need to break the **Cl-F bond** in the reactants?

**A:** No, we just need to form two more **Cl-F bonds** in the products.

$$\Delta H_{\text{rxn}} \approx \sum \Delta H (\text{bonds broken in reactants}) - \sum \Delta H (\text{bonds formed in products})$$

$$= (1 \text{ mol} \times \Delta H_{\text{F-F}}) - (2 \text{ mol} \times \Delta H_{\text{Cl-F}})$$

$$= (1 \text{ mol} \times 155 \frac{\text{kJ}}{\text{mol}}) - (2 \text{ mol} \times 256 \frac{\text{kJ}}{\text{mol}})$$

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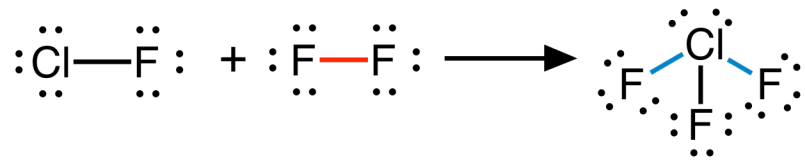
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**A:** No, we just need to form two more Cl-F bonds in the products.

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$$= (1 \text{ mol} \times \Delta H_{\text{F-F}}) - (2 \text{ mol} \times \Delta H_{\text{Cl-F}})$$

$$= (1 \text{ mol} \times 155 \frac{\text{kJ}}{\text{mol}}) - (2 \text{ mol} \times 256 \frac{\text{kJ}}{\text{mol}})$$

$$\Delta H_{\text{rxn}} \approx -357 \text{ kJ}$$

From Hess's Law  $\Delta H_{\text{rxn}} = -139.2 \text{ kJ}$ .

So what happened? Bond enthalpies are averaged, so they aren't the most accurate!

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