

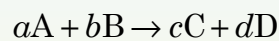
# Heats of Reaction, Formation, and Combustion

E82 – Enthalpies associated with reactions.

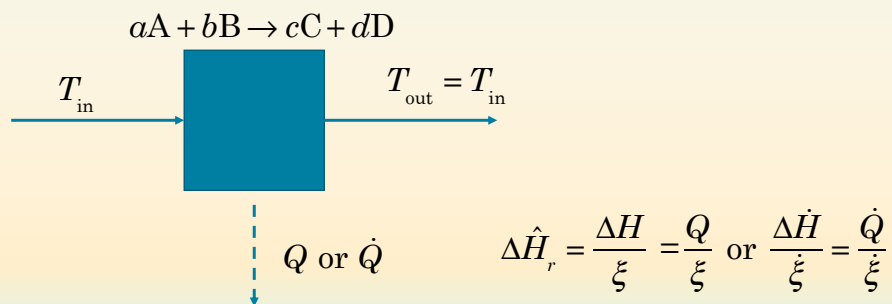
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If we have a chemical reaction, such as



We can run it in an isothermal chemical reactor, either as an open steady-state system or as a closed constant-pressure system.



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The *heat of reaction* or *enthalpy of reaction* depends on how you write the chemical equation. If you double the stoichiometric coefficients, you double the heat of reaction.

The heat of reaction is a function of temperature. At the standard reference temperature (25 °C for E82), the heat of reaction is the *standard heat of reaction*.

To calculate the heat of reaction at a temperature other than the standard temperature, you have to take into account any sensible heat changes and any phase changes since  $H$  is a state function.

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## Heat of Formation

The *heat of formation* or *enthalpy of formation* is the standard heat of reaction for forming one mole of product, starting from pure elements at their standard form of aggregation at  $T_{ref}$ . For example, the standard states at 25 °C for oxygen and nitrogen are the diatomic gases  $O_2(g)$  and  $N_2(g)$ . The standard heat of formation for any element in its standard form of aggregation is 0 by definition.

You can calculate the standard heat of reaction for any reaction as the sum of the heats of formation times the stoichiometric coefficients. Don't forget phase changes.

$$\Delta H_r^\circ = \sum v_i \Delta H_{f,i}^\circ$$

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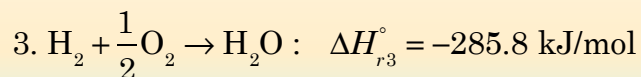
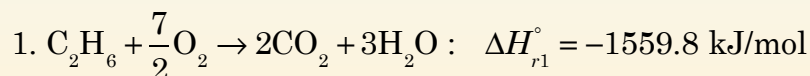
## Hess's Law



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The energetics of any reaction can be calculated by algebraically adding together any set of reactions that gives you the same overall reaction as the one you want.

Example 9.2-1 from FRB.



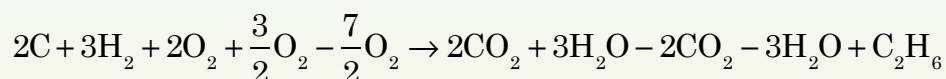
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Add 2 Equation 2's to 3 Equation 3's and subtract 1 Equation 1.



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$$\Delta H_{r4}^\circ = 2\Delta H_{r2}^\circ + 3\Delta H_{r3}^\circ - \Delta H_{r1}^\circ = 2(-393.5) + 3(-285.8) - (-1559.8) = -84.6 \text{ kJ/mol}$$

which is also the heat of formation for ethane.

If you use different sets of equations to calculate the same final equation with Hess's law, you may find that rounding and truncation errors keep the results from being identical. In the back of FRB, the heat of formation for ethane is  $-84.67 \text{ kJ/mol}$ .

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FRB uses units of kJ or Btu for heats of reaction and heats of formation. I use kJ/mol or Btu/lb-mol. Why the difference? FRB feels that including the basis confuses students. I feel that since

$$\Delta H = \xi \Delta \hat{H}_r$$

and

$$\Delta \dot{H} = \dot{\xi} \Delta \hat{H}_r$$

and the units of extent are moles, and the rate of extent are moles/time, including the basis makes perfect sense.



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### The Heat of Combustion

If you have a combustion reaction for a given species, as discussed in the Combustion Reactions video, the heat of reaction for complete combustion of one mole of fuel is called the *heat of combustion*. As a reminder, for the principal species and complete combustion, the combustion products are CO<sub>2</sub>, H<sub>2</sub>O, and SO<sub>2</sub>. CO<sub>2</sub> and SO<sub>2</sub> are gases at standard conditions. What about water?

The accepted convention is to assume water is liquid at 25 °C and 1 atm.



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