What is a Mole Reaction

When we report a reaction's change in enthalpy, ΔH, we include units of kilojoules per mole, kJ/mol. But to which species does the mol in kJ/mol refer? One of the reactants? One of the product? It is easy to visualize a mole of carbon—just weigh out 12.01 g and there you have it, a mole of carbon. But what is a mole for a reaction? To help us think through this we introduce the unit mol_{rxn} as a substitute for *mol* in kJ/*mol*.[1]

Let's see how this works. Suppose you and a classmate perform separate calorimetry experiments to determine ΔH for the reaction

$$\text{A} + 2\text{B} \longrightarrow 3\text{C}$$

Your classmate performs the experiment using 0.75 mol of A and 1.00 mol of B, and finds that q_{rxn} is –1000 kJ. She calculates ΔH by dividing q_{rxn} by the moles of limiting reagent (in this case B), obtaining

$$\Delta H = \frac{q_{\text{rxn}}}{\text{mol B}} = \frac{-1000\ \text{kJ}}{1\ \text{mol B}} = -1000\ \text{kJ/mol B}$$

You, on the other hand, perform the experiment using 0.75 mol of A and 3.00 mol of B, and find that q_{rxn} is –1500 kJ. Because A is the limiting reagent you report ΔH as

$$\Delta H = \frac{q_{\text{rxn}}}{\text{mol A}} = \frac{-1500\ \text{kJ}}{0.75\ \text{mol A}} = -2000\ \text{kJ/mol A}$$

Both results are correct even though their respective numerical values are different; however, it is inconvenient if the value we report for ΔH depends on the identity of limiting reagent.[2] If we multiply each value of ΔH by the limiting reagent's stoichiometry in the balanced reaction

$$\left[\frac{-1000\ \text{kJ}}{\text{mol B}} \times \frac{2\ \text{mol B}}{\text{mol}_{\text{rxn}}}\right] = \frac{-2000\text{kJ}}{\text{mol}_{\text{rxn}}} = \left[\frac{-2000\text{kJ}}{\text{mol A}} \times \frac{1\ \text{mol A}}{\text{mol}_{\text{rxn}}}\right]$$

then we obtain the same value for ΔH of $-2000\ \text{kJ/mol}_{\text{rxn}}$ where mol_{rxn} indicates that the value of ΔH is reported for the reaction, not for particular reactant. Note that the conversion factors $\frac{2\ \text{mol B}}{\text{mol}_{\text{rxn}}}$ and $\frac{1\ \text{mol A}}{\text{mol}_{\text{rxn}}}$ make explicit the relationship between each reactant's stoichiometry and the reaction's enthalpy.

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[1] The unit mol_{rxn} is borrowed from the textbook *Chemistry: Structure and Dynamics* by Spencer, Bodner, and Rickard.

[2] The problem here is that we ultimately want to compile tables of ΔH values. This is easy to do if each reaction has a single value for ΔH, but is more cumbersome if each reaction has two or more values for ΔH.