where $n_i - n_{i0} = \delta n_i$ is the change in the moles of species i by reaction from its initial number n_{i0}. Solving for n_i, the moles of species i after reaction is

$$n_i = n_{i0} + \xi \nu_i. \tag{14.4}$$

The total number of moles is calculated by summing this equation over all species:

$$n = n_0 + \xi \nu, \tag{14.5}$$

where n_0 and n are the total moles before and after the reaction, and ν is the sum of the stoichiometric coefficients, defined in eq. (14.2). Finally, the mole fraction of species i after the reaction is

$$x_i = \frac{n_i}{n} = \frac{n_{i0} + \xi \nu_i}{n_0 + \xi \nu}. \tag{14.6}$$

These equations demonstrate the usefulness of the extent of reaction. While the number of moles of all species changes during reaction, these changes are interrelated through a common variable, the extent of reaction. If the extent of reaction is known, all compositions can be calculated. The extent of reaction is a measure of how far the reaction has proceeded. If it is positive, it indicates that the reaction has advanced from left to right; if negative, it indicates that the reaction has advanced from right to left. Although we will be referring to the species on the left as "reactants" and those on the right as "products," these terms should be understood to be by convention. The actual direction of the chemical reaction would be indicated by the sign of the reaction extent.

Example 14.1: Extent of Reaction

A reactor contains an equimolar mixture of hydrogen, nitrogen, and ammonia under conditions that reaction (14.1) can take place. Determine the possible values of the extent of reaction and the composition (mole fractions) of the mixture ~~when the moles of ammonia have doubled over the initial value~~. when the reaction has produced 0.5 mol of ammonia.

Solution We construct the stoichiometric table below:

	H_2	N_2	NH_3
ν_i	$-\frac{3}{2}$	$-\frac{1}{2}$	1
n_{i0}	1	1	1
n_i	$1 - \frac{2\xi}{3}$	$1 - \frac{\xi}{3}$	$\xi + 1$

If the reaction proceeds to completion from left to right, the maximum value of ξ is

3 ξ/2 ξ/2

$$\xi_{\max} = \frac{3}{2},$$

2/3

because at this point one of the reactants (hydrogen) is fully consumed. If the reaction proceeds to completion from right to left, the reaction will stop when all ammonia is consumed, that is,

$$\xi_{\text{min}} = -1.$$

Therefore, the range of possible values of ξ is

$$-1 \le \xi \le 1.5.$$ 2/3

has produced 0.5 mol

If the reaction proceeds from right to left until the reactor ~~contains 2 mol~~ of ammonia, then

$$n_{\text{NH}_3} = \xi + 1 = \cancel{2} \quad \Rightarrow \quad \xi = \cancel{1}.$$ 0.5

1.5

From the stoichiometric table,

$$n_{\text{H}_2} = \cancel{0.333}, \quad n_{\text{N}_2} = \cancel{0.666}, \quad n_{\text{H}_2} = \cancel{2},$$

0.25 0.75 1.5

and the total number of moles is 3. The corresponding mole fractions are

$$x_{\text{H}_2} = \cancel{0.111}, \quad x_{\text{N}_2} = \cancel{0.222}, \quad x_{\text{H}_2} = \cancel{0.667}.$$

0.1 0.3 0.6

Comments The value of the reaction extent depends on the chosen stoichiometry but the mol fractions are independent of that choice. You should confirm this by repeating the calculation with different stoichiometric coefficients.

14.2 Standard Enthalpy of Reaction

A chemical reaction that proceeds to completion is a process whose initial state consists of all reactants and its final state of all products. This process is accompanied by a change in enthalpy, which is given by the difference between products and reactants:

$$\Delta H_{\text{rxn}} = H_{\text{products}} - H_{\text{reactants}}.$$

The precise value of this difference depends on various process details such as the temperature of reactants, whether reactants are mixed before entering the reactor or fed as pure components, whether the reaction product is delivered as a mixture or is separated into its pure components, etc. To avoid such ambiguities and to facilitate tabulations of reaction properties, we adopt a *standard* state for each component in the reaction and report all reaction properties based on these states. The following standard states are in use:

> *Standard state for gases (g):* It is defined as the pure substance *in the ideal-gas state* at 1 bar.