GIBBS FREE ENERGY IN CHEMICAL REACTIONS

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Reference: Daniel V. Schroeder, *An Introduction to Thermal Physics*, (Addison-Wesley, 2000) - Problem 5.2.

The Gibbs free energy is defined as

$$G \equiv U - TS + PV = H - TS \tag{1}$$

The enthalpy H is the total energy required to create the system from nothing, in which the environment at constant pressure P must be pushed back to create the volume V in which the new system is to be stored.

For a process occurring at constant temperature and pressure, the change in G is

$$\Delta G = \Delta H - T\Delta S \tag{2}$$

We can calculate changes in G for a process such as a chemical reaction by considering the values for the reactants. Consider the reaction in which nitrogen and hydrogen combine to form ammonia:

$$\mathrm{N_2 + 3H_2 \rightarrow 2NH_3} \tag{3}$$

We can look up the relevant values in Schroeder's book, where he gives values for 1 mole at $T = 298$ K and a pressure of 1 bar. The tabulated values are

	ΔH (kJ)	S (J K^{-1})
N_2	0	191.61
H_2	0	130.68
NH_3	-46.11	192.45

For the reaction 3 we combine 1 mole of N_2 with 3 moles of H_2 to get 2 moles of NH_3, so we have

$$\Delta H = -92.22 \times 10^3 \text{ J} \tag{4}$$

$$\Delta S = 2 \times 192.45 - 3 \times 130.68 - 191.61 \tag{5}$$

$$= -198.75 \text{ J K}^{-1} \tag{6}$$

$$\Delta G = \Delta H - T\Delta S \tag{7}$$

$$= -32.99 \times 10^3 \text{ J} \tag{8}$$

This value is for 2 moles, so for one mole of NH_3 we have

$$\Delta G = -16.5 \text{ kJ} \tag{9}$$

which is close to the value of -16.45 kJ given in Schroeder's table. (I'm not sure if we're supposed to be able to get closer with the given data.)