

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

$$(0.1) \quad G \equiv U - TS + PV = H - TS$$

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

$$(0.2) \quad \Delta G = \Delta H - T \Delta S$$

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:



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 0.3 we combine 1 mole of N₂ with 3 moles of H₂ to get 2 moles of NH₃, so we have

$$(0.4) \quad \Delta H = -92.22 \times 10^3 \text{ J}$$

$$(0.5) \quad \Delta S = 2 \times 192.45 - 3 \times 130.68 - 191.61$$

$$(0.6) \quad = -198.75 \text{ J K}^{-1}$$

$$(0.7) \quad \Delta G = \Delta H - T\Delta S$$

$$(0.8) \quad = -32.99 \times 10^3 \text{ J}$$

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

$$(0.9) \quad \Delta G = -16.5 \text{ kJ}$$

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.)