

ENTROPY OF DIAMOND AND GRAPHITE

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Reference: Daniel V. Schroeder, *An Introduction to Thermal Physics*, (Addison-Wesley, 2000) - Problems 3.30 - 3.31.

In a quasistatic process, the relation between entropy, temperature and the heat flow is

$$(0.1) \quad dS = \frac{Q}{T}$$

where Q is the (infinitesimal) amount of heat flowing into or out of the system at temperature T . For a process at constant pressure but changing temperature, Q can be written in terms of the heat capacity C_P at constant pressure, since the amount of heat required to change the temperature by dT is $C_P dT$. In that case, the entropy change between temperatures T_i and T_f is

$$(0.2) \quad \Delta S = \int_{T_i}^{T_f} \frac{C_P(T)}{T} dT$$

Example 1. From Schroeder's Figure 1.14, we can estimate a linear relation for C_P for a mole of diamond between $T = 300$ K and $T = 400$ K. Reading off the graph we get

$$(0.3) \quad C_P(300) = 6.5 \text{ J K}^{-1}$$

$$(0.4) \quad C_P(400) = 11 \text{ J K}^{-1}$$

Between these temperatures, a formula for $C_P(T)$ is therefore a straight line:

$$(0.5) \quad \frac{C_P(T) - 6.5}{T - 300} = \frac{11 - 6.5}{400 - 300} = 0.045$$

$$(0.6) \quad C_P(T) = 0.045T - 7$$

If we assume this is valid over the range of temperature from 298 K up to 500 K, we can get the entropy change over that range for a mole of diamond (incidentally, if you want to try this experiment, you'll need a very big diamond. A mole of diamond (carbon) is around 12 grams, and there are

5 carats per gram, so you're looking for a 60 carat diamond). The entropy change is

$$(0.7) \quad \Delta S = \int_{298}^{500} \frac{0.045T - 7}{T} dT$$

$$(0.8) \quad = [0.045T - 7 \ln T]_{298}^{500}$$

$$(0.9) \quad = 5.47 \text{ J K}^{-1}$$

The entropy of a mole of diamond at $T = 298 \text{ K}$ is given in Schroeder's appendix as 2.38 J K^{-1} so the total entropy at $T = 500 \text{ K}$ is

$$(0.10) \quad S(500) = 2.38 + 5.47 = 7.85 \text{ J K}^{-1}$$

Example 2. An empirical formula obtained by fitting to measured data for C_P for one mole of graphite is

$$(0.11) \quad C_P = a + bT - \frac{c}{T^2}$$

where the constants are

$$(0.12) \quad a = 16.86 \text{ J K}^{-1}$$

$$(0.13) \quad b = 4.77 \times 10^{-3} \text{ J K}^{-2}$$

$$(0.14) \quad c = 8.54 \times 10^5 \text{ J K}$$

The entropy change of a mole of graphite over the range of temperature from 298 K up to 500 K is therefore

$$(0.15) \quad \Delta S = \int_{298}^{500} \frac{a + bT - \frac{c}{T^2}}{T} dT$$

$$(0.16) \quad = \left[a \ln T + bT + \frac{c}{2T^2} \right]_{298}^{500}$$

$$(0.17) \quad = 6.59 \text{ J K}^{-1}$$

Adding on the tabulated value for $T = 298 \text{ K}$ we get

$$(0.18) \quad S(500) = 5.74 + 6.59 = 12.33 \text{ J K}^{-1}$$

The entropy of graphite is larger than that of diamond which we'd expect since diamond's crystal structure is more ordered than that of graphite.

PINGBACKS

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