Making diamond from graphite

The free energy of formation of diamond is:

C(s, graphite) **->** C(s, diamond) $\Delta_r G^o = + 2.90$ kJ/mol

and the densities are:

ρ(graphite) = 2.26 and ρ(diamond) = 3.51 (grams/cm^3)

Calculate the pressure required to transform carbon into ultra-pure industrial diamond with a purity of 99.999%. Assume that this means that the mole fraction of the diamond is 0.99999 and that of graphite is 0.00001.

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Solution: The first step is to calculate ΔG.

$$\Delta G = \Delta G^0 + RT\ lnQ$$

$$\Delta G = 2900 + (8.31)(298)\ ln\left(\frac{0.99999}{0.00001}\right)$$

$$\Delta G = 2900 + (8.31)(298)\ (11.51)$$

$$\Delta G = 31{,}400\ J/mol$$

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The free energy of the applied pressure must negative and equal to the positive free energy o formation. It is calculated from the pressure dependence, $\Delta G = \Delta V_m(P_2 - P_1)$.

$$\Delta V_m = \frac{M_m}{\rho_d} - \frac{M_m}{\rho_g}$$

$$\Delta V_m = \frac{0.012\ kg/mol}{3510\ kJ/m^3} - \frac{0.012\ kg/mol}{2260\ kJ/m^3}$$

$$\Delta V_m = -1.89\ x\ 10^{-6}$$

$$P_2 = P_1 + \frac{\Delta G}{\Delta V_m}$$

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The calculate free energy must be achieved based on the pressure dependence:

$$\Delta V_m = -1.89\ x\ 10^{-6}\ m^3/mol$$

$$P_2 = 10^5\ Pa + \frac{-31400\ J/mol}{-1.89\ x\ 10^{-6}\ m^3/mol}$$

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$$P_2 = 1.64\ x\ 10^{10}\ Pa$$

$$P_2 = 1.64\ x\ 10^5\ bar$$