

## Ex.1

In[152]:=  $g := \text{Earth}_{\text{PLANET}} [\text{gravity}] \checkmark ;$

$\rho := \text{water}_{\text{CHEMICAL}} [\text{mass density}] \dots \checkmark$

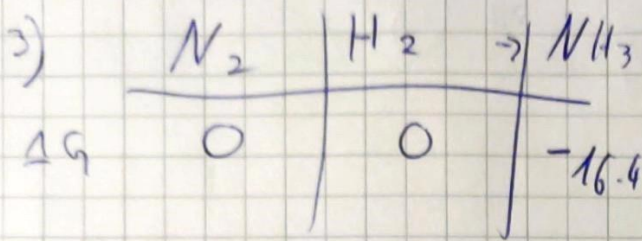
$T := 298 \text{ K} \dots \checkmark ; \Delta h := 1.2 \text{ cm} \checkmark$

$R := R \dots \checkmark ; m := 3 \text{ g/L} \dots \checkmark$

$$\Delta p = \rho * g * \Delta h$$

$$M = m (R * T) / (\Delta p) \quad // \text{UnitConvert}$$

Out[155]=  $1172.53 \text{ g/ (cm s}^2\text{)}$



$$\rightarrow \Delta G = -32.8 \frac{kJ}{mol}$$

$$n_{H_2} = n_{N_2} \Rightarrow P_{H_2} = P_{N_2}$$

$$P_{NH_3} = \frac{\sqrt{K} P_{H_2}^2}{P_0}$$

$$1 \text{ atm} = P_{N_2} + P_{H_2} + P_{NH_3} = 2P_{H_2} + \frac{\sqrt{K} P_{H_2}^2}{P_0}$$

$$\Rightarrow P_{H_2} \approx \pm 0.035 \text{ atm} \Rightarrow P_{NH_3} = 1 \text{ atm} - 2 \cdot P_{H_2} \approx 0.93 \text{ atm}$$

b)

$$P_{H_2} = \frac{PV}{nRT} = \frac{2 \cdot 10^{-2} \cdot 10^5}{0.2 \cdot 8.314 \cdot 298} = 4.0 \text{ atm}$$

$$P_{NH_3} = \frac{5.54 \cdot 10^{-2} \cdot 10^5}{0.2 \cdot 8.314 \cdot 298} = 1.13 \text{ atm}$$

$$PV = nRT \quad \Delta P_{NH_3} = \frac{0.2 \text{ mol} \cdot R \cdot T}{V} \approx 0.2 \text{ atm}$$

$$\Rightarrow P_{H_2} = P_{N_2} = 0.035 \text{ atm}, P_{NH_3} = 1.13 \text{ atm}$$

neues Gleichgewicht bei  $P_{H_2}^{neu} = P_{H_2} + 3x$

$$K = \frac{P_{NH_3}^2 \cdot P_0^2}{P_{N_2}^2 \cdot P_{H_2}^2} = \frac{(P_{NH_3} - 2x)^2 P_0^2}{(P_{N_2} + 3x)^2 (P_{H_2} + x)^2} \Rightarrow x \approx 0.0015 \text{ atm}$$

$$P_{H_2}^{neu} = P_{H_2} + x$$

$$P_{NH_3}^{neu} = P_{NH_3} + 2x$$

$$\Rightarrow P_{N_2}^{neu} = 0.0365 \text{ atm} \quad P_{H_2}^{neu} \approx 0.0395 \text{ atm} \quad P_{NH_3}^{neu} \approx 0.927 \text{ atm}$$

c)

$$P_{H_2}^{neu} = 0.07 \text{ atm} + 3x$$

$$P_{N_2}^{neu} = 0.07 \text{ atm} + x$$

$$\Rightarrow x \approx 0.008 \text{ atm}$$

$$P_{NH_3}^{neu} = 1.86 \text{ atm} - 2x$$

$$\Rightarrow P_{N_2}^{neu} \approx 0.064 \text{ atm} \quad P_{H_2}^{neu} \approx 0.046 \text{ atm} \quad P_{NH_3}^{neu} \approx 1.876 \text{ atm}$$

Reaktion läuft unter Druck "besser" ab, Gleichgewicht verschiebt sich richtung Produkt.



$$Z_A = \frac{z_A^{N_A}}{N_A!}$$

$$Z_{AB} = Z_A Z_B$$

$$Z_A = \frac{V}{\lambda_A^3}$$

$$F = -k_B T \ln Z = -k_B T (\ln Z_A + \ln Z_B)$$

$$= -k_B T (N_A \ln \left( \frac{V}{\lambda_A^3} \right) + N_A \ln N_A + N_A + N_B \ln \left( \frac{V}{\lambda_B^3} \right) + N_B \ln N_B + N_B)$$

$$= -k_B T (N_A \ln \left( \frac{V}{\lambda_A^3} \right) + N_A + N_B \ln \left( \frac{V}{\lambda_B^3} \right) + N_B)$$

$$= -k_B T [N_A (\ln \left( \frac{Z_A}{N_A} \right) + 1) + N_B (\ln \left( \frac{Z_B}{N_B} \right) + 1)]$$

$$S = - \frac{\partial F}{\partial T} = - \frac{\partial F_A}{\partial T} - \frac{\partial F_B}{\partial T}$$

$$\frac{\partial F_A}{\partial T} = - \frac{F_A}{T} + k_B T N_A \frac{\partial}{\partial T} (\ln(Z_A) - \ln(N_A) + 1) =$$

$$= - \frac{F_A}{T} + k_B T N_A \frac{\partial \ln(Z_A)}{\partial T} =$$

$$= - \frac{F_A}{T} + k_B T N_A \frac{1}{Z_A} \gamma^{\frac{5}{2}} T^{\frac{3}{2}} =$$

$$= + k_B N_A (\ln(Z_A) - \ln(N_A) + 1) + \frac{5 k_B T N_A}{2 Z_A} \frac{V}{\lambda^3}$$

$$= k_B N_A (\ln \left( \frac{Z_A}{N_A} \right) + \frac{5}{2})$$

$$S = S_A + S_B = k_B [N_A (\ln \left( \frac{Z_A}{N_A} \right) + \frac{5}{2}) + N_B (\ln \left( \frac{Z_B}{N_B} \right) + \frac{5}{2})]$$

$$U = F + ST \quad U_A = F_A + S_A T = -k_B T N_A (\ln \left( \frac{Z_A}{N_A} \right) + 1) + k_B T N_A (\ln \left( \frac{Z_A}{N_A} \right) + \frac{5}{2}) = \frac{3}{2} N_A k_B T$$

$$U = U_A + U_B = \frac{3}{2} k_B T (N_A + N_B)$$

$$P = - \frac{\partial F}{\partial V} \quad P_A = - \frac{\partial F_A}{\partial V} = + k_B T N_A \frac{\partial}{\partial V} (\ln(V) - \ln(\lambda_A^3) + 1) = \frac{k_B T N_A}{V}$$

$$P = \frac{k_B T}{V} (N_A + N_B)$$

$$H = U + PV \quad H_A = \frac{3}{2} N_A k_B T + k_B T N_A = \frac{5}{2} k_B T N_A \quad H = \frac{5}{2} k_B T (N_A + N_B)$$



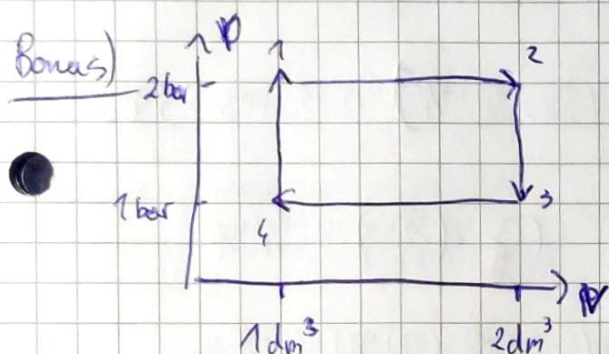
$$G = F + pV \quad G_A = -k_B T N_A (\ln(\frac{z_A}{N_A}) + 1) + k_B T N_A = -k_B T N_A \ln(\frac{z_A}{N_A})$$

$$G = -k_B T [N_A \ln(\frac{z_A}{N_A}) + N_B \ln(\frac{z_B}{N_B})]$$

$$C_V = \left( \frac{\partial U}{\partial T} \right)_{V, N}$$

$$C_V^A = \frac{3}{2} N_A k_B$$

$$C_V = \frac{3}{2} (N_A + N_B) k_B$$



$$T = \frac{pV}{Nk_B}$$

$$C_V = \frac{5}{2} N k_B$$

$$C_V T = \frac{5}{2} pV$$

$$\Delta W_{12} = \int_1^2 p dV = -2 \text{ bar} \cdot 1 \text{ dm}^3 = -\Delta Q_{12}$$

$$\Delta Q_{23} = C_V (T_3 - T_2) = \frac{5}{2} (-2) \text{ bar} \cdot \text{dm}^3 = -5 \text{ bar} \cdot \text{dm}^3$$

$$\Delta W_{34} = +1 \text{ bar} \cdot 1 \text{ dm}^3$$

$$\Delta Q_{41} = C_V (T_1 - T_4) = \frac{5}{2} \text{ bar} \cdot \text{dm}^3$$

$$\eta = \frac{\Delta W_{12} + \Delta W_{34}}{\Delta Q_{23} + \Delta Q_{41}} = \frac{-1 \text{ bar} \cdot \text{dm}^3}{-5 \text{ bar} \cdot \text{dm}^3} = \frac{2}{5}$$

Es geht viel Energie in Wärme verloren, Isotherme und adiabatische Prozesse sind da besser (wie im Carnot Zyklus).