Ex.1

```
In[152]:= g := Earth PLANET [gravity] ;

ρ := water CHEMICAL [mass density]

T := 298 K ; Δh := 1.2 cm

R := R ; m := 3 g/L

Δp = ρ*g*Δh
M = m (R*T) / (Δp) // UnitConvert

Out[155]= 1172.53 g/(cm s^2)
```

✓

3)

	N_2	H_2	$\rightarrow NH_3$
ΔG	0	0	-16.4

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

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

$p_{NH_3} = \frac{\sqrt{K}\, p_{H_2}^2}{p_0}$

$1\,atm = p_{N_2} + p_{H_2} + p_{NH_3} = 2p_{H_2} + \frac{\sqrt{K}\, p_{H_2}^2}{p_0}$

$\Rightarrow p_{H_2} \overset{!}{\approx} 0.035\,atm \Rightarrow p_{NH_3} = 1\,atm - 2 \cdot p_{H_2} \approx 0.93\,atm$

b)

$\cancel{A_{H_2}\; n_{N_2} = \frac{pV}{RT} = 2 \cdot 10^{22} \quad A_{NH_3} = 5.59 \cdot 10^{23}}$

$pV = N k_B T \qquad \Delta p_{NH_3} = \frac{0.2\,mol\; RT}{V} \approx 0.2\,atm$

$\Rightarrow p_{H_2} = p_{N_2} \overset{=0{,}035\,atm}{}, \; p_{NH_3} = 1.13\,atm$, neues Gleichgewicht bei $p_{H_2}^{neu} = p_{H_2} + 3x$

$p_{N_2}^{neu} = p_{N_2} + x$

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

$K = \frac{p_{NH_3}^2 \cdot p_0^2}{p_{N_2}^3 p_{H_2}} = \frac{(p_{NH_3} - 2x)^2\, p_0^2}{(p_{H_2} + 3x)^3 (p_{N_2} + x)} \Rightarrow x \approx 0{,}0015\,atm$

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

c) $p_{H_2}^{neu} = 0.07\,atm + 3x$

$p_{N_2}^{neu} = 0.07\,atm + x \qquad \Rightarrow x \approx 0.008\,atm$

$p_{NH_3}^{neu} = 1.86\,atm - 2x$

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

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

) $Z_A = \frac{z_A^{N_A}}{N_A!}$ $\quad Z_{AB} = Z_A Z_B$ $\quad z_A = \frac{V}{\lambda_A^3}$

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

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

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

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

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

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

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

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

$$= + k_B N_A \left(\ln(z_A) - \ln(N_A) + 1 \right) + \frac{5 k_B T N_A}{2 \, z_A} T^{\frac{3}{2}} \frac{V}{\lambda_A^3}$$

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

$z_A = \frac{V}{\lambda_A^3}$, $\lambda_A = \hbar \sqrt{\frac{2\pi}{m k_B T}} = \alpha (T)^{-\frac{1}{2}}$

$$z_A = \frac{\frac{N k_B T}{p}}{\left(\alpha (T)^{-\frac{1}{2}}\right)^3} =$$

$= \gamma T^{5/2}$, $\gamma = \frac{N_A k_B \sqrt{m k_B}^3}{p \hbar^3 \sqrt{2\pi}^3}$

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

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

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

$p = -\frac{\partial F}{\partial V}$ $\quad p_A = -\frac{\partial F_A}{\partial V} = + k_B T N_A \frac{\partial}{\partial V} \left(\ln(V) - \ln(\lambda_A^3 N_A) + 1 \right) = \frac{k_B T N_A}{V}$

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

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

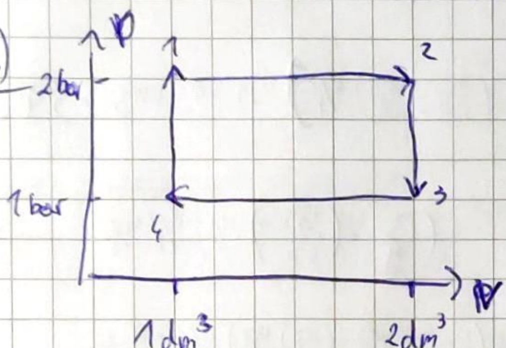
$G = F + pV$ $\qquad G_A = -k_B T N_A \left(\ln\left(\frac{Z_A}{N_A}\right) + 1\right) + k_B T N_A = -k_B T N_A \ln\left(\frac{Z_A}{N_A}\right)$

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

$C_V = \left(\frac{\partial U}{\partial T}\right)_{V,N}$ $\qquad C_V^A = \frac{3}{2} N_A k_B$

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

Bonus)



$T = \frac{pV}{N k_B}$

$C_V = \frac{5}{2} N k_B \qquad C_V T = \frac{5}{2} pV$

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

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

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

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

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

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

$$F = -k_B T \ln Z = -k_B T \left[\ln\left(\frac{z_A^{N_A}}{N_A!}\right) + \ln\left(\frac{z_B^{N_B}}{N_B!}\right) \right] = -k_B T \left(N_A \ln(z_A) - N_A \ln N_A + N_A + N_B \ln(z_B) + N_B - N_B \ln N_B \right)$$

$$= \cancel{k_B T} \frac{N_A}{N_A+N_B} F_A + \frac{N_B}{N_A+N_B} F_B + k_B T (N_A+N_B)(x_A \ln x_A + x_B \ln x_B)$$

$$x_A = \frac{N_A}{N_A+N_B}$$

$$= x_A F_A + x_B F_B + N k_B T \left[x_A \ln x_A + x_B \ln x_B \right]$$

$$S = -\left(\frac{\partial F}{\partial T}\right)_V = k_B \ln Z + k_B T \left(\frac{\partial \ln(Z)}{\partial T}\right)_V = k_B \ln\left[N_A \ln z_A - N_A \ln N_A + N_A + N_B \ln z_B - N_B \ln N_B + N_B \right] + k_B T \left(\frac{\partial \ln z_A}{\partial T} + \frac{\partial \ln z_B}{\partial T} \right)$$

$$= x_A \left(\frac{\partial F_A}{\partial T}\right)_V + x_B \left(\frac{\partial F_B}{\partial T}\right)_V - N k_B (x_A \ln x_A + x_B \ln x_B) = x_A S_A + x_B S_B - N k_B (x_A \ln x_A + x_B \ln x_B)$$

$$U = k_B T^2 \left(\frac{\partial \ln Z}{\partial T}\right)_{N,V} = k_B T^2 \frac{\partial}{\partial T}\left(\ln(z_A) + \ln(z_B)\right) = k_B T^2 \frac{\partial \ln z_A}{\partial T} + k_B T^2 \frac{\partial \ln z_B}{\partial T} = U_A + U_B$$

$$p = -\left(\frac{\partial F}{\partial V}\right)_{N,T} = \cancel{-k_B T \left(\frac{\partial \ln}{\partial V}\right)} - k_B T \frac{1}{Z} \left(\frac{\partial Z}{\partial V}\right)_{N,T} = -k_B T \frac{1}{z_A z_B} \left(\frac{\partial z_A}{\partial V} z_B + \frac{\partial z_B}{\partial V} z_A \right) = p_A + p_B$$

$$H = U + pV = k_B T^2 \left(\frac{\partial \ln Z}{\partial T}\right)_{N,V} - k_B T V \left(\frac{\partial \ln Z}{\partial V}\right)_{N,T} = U_A + p_A V + U_B + p_B V = H_A + H_B$$

$$G = H - TS = x_A (H_A - T S_A) + x_B (H_B - T S_B) + N k_B T (x_A \ln x_A + x_B \ln x_B) = x_A G_A + x_B G_B + N k_B T (x_A \ln x_A + x_B \ln x_B)$$

$$C_V = \left(\frac{\partial H}{\partial T}\right)_V = \frac{\partial}{\partial T}\left(k_B T^2 \left(\frac{\partial \ln Z}{\partial T}\right)_{N,V} - k_B T V \left(\frac{\partial \ln Z}{\partial T}\right)_{N,T} \right)_V = x_A \left(\frac{\partial H_A}{\partial T}\right)_V + x_B \left(\frac{\partial H_B}{\partial T}\right)_V = x_A C_{VA} + x_B C_{VB}$$

Korrektur $\widehat{=}$ x. 4

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