

# Zbirka rešenih nalog iz Fizikalne kemije I

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## A) Enačbe stanja in plinski zakoni

1) Živosrebrni termometer meri temperaturo od 0 do 50 °C. Jakec ne želi v šolo ter posledično naredi še eno neumnost – s pomočjo lučke ga pregreje na 51 °C. Za koliko pri tem naraste tlak v notranjosti živosrebrnega termometra?

Iz grafa priloženega na koncu zbirke pri nizkih tlakih najprej odčitamo koeficienta  $\alpha$  in  $\kappa$  za živo srebro:

$$\alpha = 1,8 \cdot 10^{-4} \text{ K}^{-1}$$

$$\kappa = 3,9 \cdot 10^{-6} \text{ bar}^{-1}$$

$$\begin{aligned}\left(\frac{\partial P}{\partial T}\right)_V &= \frac{\alpha}{\kappa} = 46 \frac{\text{bar}}{\text{K}} \\ \left(\frac{\partial P}{\partial T}\right)_V &\approx \left(\frac{\Delta P}{\Delta T}\right)_V \\ \Delta T = 1 \text{ K} \Rightarrow \Delta P &= \left(\frac{\partial P}{\partial T}\right)_V \Delta T = 46 \text{ bar}\end{aligned}$$

2) S pomočjo van der Waalsove enačbe izračunajte volumen 0,454 kg acetilena pri tlaku 34 bar ter temperaturi 18 °C.

$$b = 51,2 \text{ mL mol}^{-1}$$

$$a = 4,46 \cdot 10^6 \text{ bar mL}^2 \text{ mol}^{-2}$$

Acetilen ima molekulsko formulo C<sub>2</sub>H<sub>2</sub> ter M=26 g/mol.

$$n = \frac{m}{M} = 17,45 \text{ mol}$$

Volumna iz van der Waalsove enačbe ne moremo eksplisitno izraziti:

$$\left(P + a \frac{n^2}{V^2}\right)(V - bn) = nRT$$

Posledično bomo morali volumen acetilena iskati numerično kot ničlo spodnje funkcije:

$$f(V) = \left(P + a \frac{n^2}{V^2}\right)(V - bn) - nRT = 0$$

Za prvi poskus bomo uporabili volumen idealnega plina pri identičnih pogojih:

$$V = \frac{nRT}{P} = 12,4 \cdot 10^3 \text{ ml}$$

Nato izdelamo sledečo tabelo:

V [mL]	f(V) [bar mL]
$12,4 \cdot 10^3$	$0,707 \cdot 10^5$
$11 \cdot 10^3$	$0,35 \cdot 10^5$
$10 \cdot 10^3$	$0,11 \cdot 10^5$
$9 \cdot 10^3$	$-0,11 \cdot 10^5$

$f(V)$  spremeni predznak in posledično zavzame ničlo med 9 in 10 L. Posledično lahko volumen acetilena ocenimo na 9,5 L.

3) Izrazite koeficiente  $\alpha$ ,  $\beta$  in  $\kappa$  za 1 mol van der Waalsovega plina z vsemi količinami razen s tlakom. Pokažite, da je  $\beta P = \alpha/\kappa$ .

Van der Waalsov plin sledi van der Waalovi enačbi:

$$\begin{aligned} \left( P + a \frac{n^2}{V^2} \right) (V - bn) &= nRT \\ n = 1 \Rightarrow \left( P + \frac{a}{V^2} \right) (V - b) &= RT \\ P = \frac{RT}{V - b} - \frac{a}{V^2} \text{ ter } T = \frac{1}{R} \left( P + \frac{a}{V^2} \right) (V - b) \end{aligned}$$

Ker naloga prepoveduje izražanje s tlakom, moramo na mesto njega vedno vstaviti gornji levi izraz:

$$\beta = \frac{1}{P} \left( \frac{\partial P}{\partial T} \right)_V = \frac{1}{P} * \frac{R}{V - b} = \frac{RV^2}{RTV^2 - a(V - b)}$$

Ker volumna iz van der Waalsove enačbe ne moremo eksplisitno izraziti, se poslužimo dvojnega ulomka:

$$\begin{aligned} \alpha &= \frac{1}{V} \left( \frac{\partial V}{\partial T} \right)_P = \frac{1}{V} \frac{1}{\left( \frac{\partial T}{\partial V} \right)_P} = \frac{1}{V} * \frac{R}{-\frac{2a}{V^3}(V - b) + \left( P + \frac{a}{V^2} \right)} = \frac{R(V - b)V^2}{RTV^3 - 2a(V - b)^2} \\ \kappa &= -\frac{1}{V} \left( \frac{\partial V}{\partial P} \right)_T = -\frac{1}{V} \frac{1}{\left( \frac{\partial P}{\partial V} \right)_T} = -\frac{1}{V} * \frac{1}{-\frac{RT}{(V-b)^2} + \frac{2a}{V^3}} = \frac{V^2(V - b)^2}{-2a(V - b)^2 + RTV^3} \\ \beta P &= \frac{\alpha}{\kappa} \\ \frac{RV^2}{RTV^2 - a(V - b)} * \frac{RTV^2 - a(V - b)}{(V - b)V^2} &= \frac{R(V - b)V^2}{RTV^3 - 2a(V - b)^2} * \frac{-2a(V - b)^2 + RTV^3}{V^2(V - b)^2} \\ \frac{R}{(V - b)} &= \frac{R}{(V - b)} \\ 1 &= 1 \end{aligned}$$

4) Z uporabo Hagen-Watson-Ragatzovega diagrama iz priloge izračunajte volumen 1 kg O<sub>2</sub> pri -88 °C ter 45,3 bar.

$$T_K = 154,4 \text{ K}$$

$$P_K = 50,4 \text{ bar}$$

Najprej moramo izračunati reducirano temperaturo in tlak:

$$T_R = \frac{T}{T_K} = \frac{185,15 \text{ K}}{154,4 \text{ K}} = 1,2$$

$$P_R = \frac{P}{P_K} = \frac{45,3 \text{ bar}}{50,4 \text{ bar}} = 0,9$$

Z uporabo Hagen-Watson-Ragatzovega diagrama iz priloge pri gornjih vrednostih reducirane temperature in tlaka odčitamo vrednost faktorja kompresibilnosti z:

$$z = 0,8$$

$$z = \frac{PV}{nRT} \Rightarrow V = \frac{znRT}{P} = \frac{zmRT}{MP} = 8,5 \text{ L}$$

5) Za 1 mol plina, ki sledi enačbi P(V-nb)=nRT, izrazite faktor kompresibilnosti z, drugi virialni koeficient b<sub>2</sub> ter Boylovo temperaturo T<sub>B</sub>.

$$n = 1 \Rightarrow P(V - b) = RT$$

$$V = \frac{RT}{P} + b$$

$$n = 1 \Rightarrow PV_i = RT$$

$$V_i = \frac{RT}{P}$$

$$z = \frac{V}{V_i} = \frac{\frac{RT}{P} + b}{\frac{RT}{P}} = 1 + \frac{Pb}{RT}$$

$$b_2 = \lim_{P \rightarrow 0} \left( \frac{\partial z}{\partial P} \right)_T = \lim_{P \rightarrow 0} \frac{b}{RT} = \frac{b}{RT}$$

$$\lim_{P \rightarrow 0} \left( \frac{\partial z}{\partial P} \right)_{T_B} = 0 \Rightarrow T_B = \infty$$

6)  $N_2O_4$  disociira s stopnjo disociacije  $\alpha=0,185$ . Kolikšna je povprečna molska masa nastale plinske mešanice? Na koliko pri tem naraste tlak, če je njegova začetna vrednost 1,2 bar. Kolikšna sta parcialna tlaka plinov plinske mešanice? Temperatura in volumen sta konstantna.

$$N_2O_4(g) \rightleftharpoons 2NO_2(g)$$

t=0	n <sub>0</sub>	0	Σ= n <sub>0</sub>
t=∞	n <sub>0</sub> (1-α)	2α n <sub>0</sub>	Σ= n <sub>0</sub> (1+α)
$\bar{M} = \sum_i^k X_i M_i = X_1 M_1 + X_2 M_2$			
$\bar{M} = \frac{n_0(1 - \alpha)}{n_0(1 + \alpha)} M_1 + \frac{2n_0}{n_0(1 + \alpha)} M_2 = 77,6 \text{ g/mol}$			
$P_\infty = \frac{n_\infty RT}{V}$			
$P_0 = \frac{n_0 RT}{V}$			
$\frac{P_\infty}{P_0} = \frac{n_\infty}{n_0} = \frac{n_0(1 + \alpha)}{n_0} = (1 + \alpha)$			
$P_\infty = P_0(1 + \alpha) = 1,42 \text{ bar}$			
$P_1 = X_1 P_\infty = \frac{n_0(1 - \alpha)}{n_0(1 + \alpha)} P_\infty = 0,977 \text{ bar}$			
$P_2 = P_\infty - P_1 = 0,443 \text{ bar}$			

## B) Prvi zakon termodinamike

1) Posodo idealnega plina z volumnom 10 L in tlakom 25 bar odpremo. Kolikšno delo opravi plin na okolico s tlakom 1 bar, če sta temperatura plina in okolice enaka?

Začnemo z definicijo volumnskega dela:

$$W = - \int_{V_1}^{V_2} P_0 dV == - \int_{V_1}^{V_2} P_2 dV = -P_2(V_2 - V_1)$$

Ker sta temperaturi plina in okolice enaka:

$$P_1 V_1 = P_2 V_2 \Rightarrow V_2 = \frac{P_1 V_1}{P_2}$$

$$W = -P_2 \left( \frac{P_1 V_1}{P_2} - V_1 \right) = -P_1 V_1 + P_2 V_1 = (P_2 - P_1)V_1 = -24 \text{ kJ}$$

2) Izračunajte delo pri segretju 200 cm<sup>3</sup> vode pri tlaku 1 bar od 25 do 50 °C. Kolikšni sta prenesena toplota ter sprememba entalpije.

$$\alpha = 2,1 \cdot 10^{-4} \text{ K}^{-1}$$

$$\rho = 1 \text{ g/cm}^3$$

$$\overline{c_p} = 75,3 \frac{J}{\text{mol K}}$$

Začnemo z definicijo volumnskega dela:

$$W = - \int_{V_1}^{V_2} P_0 dV$$

Ker ne poznamo začetnega in končnega volumna, integracijo s pomočjo definicije  $\alpha$  prenesemo na začetno in končno temperaturo:

$$\alpha = \frac{1}{V} \left( \frac{\partial V}{\partial T} \right)_P \Rightarrow dV = \alpha V dT$$

$$W = - \int_{T_1}^{T_2} P_0 \alpha V dT = -P_0 \alpha V (T_2 - T_1) = -0,105 \text{ J}$$

Toplota prenesena pri konstantnem tlaku je enaka spremembi entalpije:

$$Q_P = \Delta H = \int_{T_1}^{T_2} n \overline{c_p} dT = \frac{\rho V}{M} \overline{c_p} (T_2 - T_1) = 20,92 \text{ kJ}$$

3) Joule-Thomsonov koeficient van der Waalsovega plina je izražen kot

$$\mu_{JT} = \frac{1}{c_P} \left( \frac{2a}{RT} - b - \frac{3abP}{R^2 T^2} \right)$$

Izpeljite izraz za inverzno temperaturo kot funkcijo tlaka.

$$\begin{aligned}\mu_{JT}(T_i) &= 0 \\ \frac{1}{c_P} \left( \frac{2a}{RT_i} - b - \frac{3abP}{R^2 T_i^2} \right) &= 0 \\ \left( \frac{2a}{RT_i} - b - \frac{3abP}{R^2 T_i^2} \right) &= 0 \\ bR^2 T_i^2 - 2aRT_i + 3abP &= 0\end{aligned}$$

Dobimo kvadratno enačbo – spomnimo se njene rešitve:

$$\begin{aligned}ax^2 + bx + c = 0 &\Rightarrow x_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \\ T_i &= \frac{2aR \pm \sqrt{4a^2 R^2 - 12ab^2 R^2 P}}{2bR^2} \\ T_i &= \frac{a}{bR} \left( 1 \pm \sqrt{1 - \frac{3b^2}{a} P} \right)\end{aligned}$$

4) Izračunajte delo pri reverzibilni a) izotermni oziroma b) adiabatni ekspanziji 2 mol idelanega plina z 10 L ter 25 °C na 20 L.

$$\overline{c_V} = \frac{5}{2} R$$

a) izotermna ekspanzija

$$W = -nRT \ln \frac{V_2}{V_1} = -3,44 \text{ kJ}$$

b) adiabatna ekspanzija

$$\overline{c_P} = \overline{c_V} + R = \frac{7}{2} R$$

$$\gamma = \frac{\overline{c_P}}{\overline{c_V}} = 1,4$$

$$W = n\overline{c_V} T_1 \left[ \left( \frac{V_2}{V_1} \right)^{\gamma-1} - 1 \right] = -3 \text{ kJ}$$

5) Izpeljite enačbo, ki povezuje začetno in končno temperaturo z začetnim in končnim volumnom, pri reverzibilni adiabatni spremembi 1 mol plina, ki sledi van der Waalsovi enačbi.

$$\bar{c_V} = A + BT$$

Van der Waalsov plin sledi van der Waalsovi enačbi:

$$\left( P + a \frac{n^2}{V^2} \right) (V - bn) = nRT$$

$$n = 1 \Rightarrow \left( P + \frac{a}{V^2} \right) (V - b) = RT \Rightarrow P = \frac{RT}{V - b} - \frac{a}{V^2}$$

Notranja energija je funkcija volumna in temperature:

$$U = f(V, T) \Rightarrow dU = \left( \frac{\partial U}{\partial V} \right)_T dV + \left( \frac{\partial U}{\partial T} \right)_V dT$$

$$\left( \frac{\partial U}{\partial T} \right)_V = \bar{c_V} = A + BT$$

Notranji tlak enega mola van der Waalsovega plina pa je enak:

$$\left( \frac{\partial U}{\partial V} \right)_T = \frac{a}{V^2}$$

$$dU = \frac{a}{V^2} dV + (A + BT) dT$$

Po drugi strani pa velja tudi prvi zakon termodinamike:

$$dU = dQ + dW$$

Pri adiabatni spremembi torej:

$$dQ = 0 \Rightarrow dU = dW = -PdV = -\frac{RT}{V-b} dV + \frac{a}{V^2} dV$$

Izenačimo spremembi notranje energije po prvem in drugem načinu:

$$dU = dU \Rightarrow \frac{a}{V^2} dV + (A + BT) dT = -\frac{RT}{V-b} dV + \frac{a}{V^2} dV$$

$$(A + BT) dT = -\frac{RT}{V-b} dV$$

Ločimo spremenljivki in integriramo:

$$\int_{T_1}^{T_2} \left( \frac{A}{T} + B \right) dT = \int_{V_1}^{V_2} -\frac{R}{V-b} dV$$

$$A \ln \frac{T_2}{T_1} + B(T_2 - T_1) = -R \ln \frac{V_2 - b}{V_1 - b}$$

6) Izrazite razliko med specifično topoto pri stalnem tlaku ter specifično topoto pri stalnem volumnu za 1 mol van der Waalsovega plina z vsemi količinami razen s tlakom.

Van der Waalsov plin sledi van der Waalovi enačbi:

$$\begin{aligned} \left( P + a \frac{n^2}{V^2} \right) (V - bn) &= nRT \\ n = 1 \Rightarrow \left( P + \frac{a}{V^2} \right) (V - b) &= RT \\ P = \frac{RT}{V - b} - \frac{a}{V^2} \text{ ter } T &= \frac{1}{R} \left( P + \frac{a}{V^2} \right) (V - b) \\ c_P - c_V &= \left[ P + \left( \frac{\partial U}{\partial V} \right)_T \right] \left( \frac{\partial V}{\partial T} \right)_P \end{aligned}$$

Ker volumna iz van der Waalsove enačbe ne moremo eksplisitno izraziti, se poslužimo dvojnega ulomka:

$$c_P - c_V = \left[ P + \left( \frac{\partial U}{\partial V} \right)_T \right] \frac{1}{\left( \frac{\partial T}{\partial V} \right)_P}$$

Notranji tlak enega mola van der Waalsovega plina pa je enak:

$$\begin{aligned} \left( \frac{\partial U}{\partial V} \right)_T &= \frac{a}{V^2} \\ c_P - c_V &= \left[ P + \frac{a}{V^2} \right] \frac{R}{-\frac{2a}{V^3}(V - b) + \left( P + \frac{a}{V^2} \right)} = \frac{R}{1 - \frac{2a(V - b)}{V^3 \left( P + \frac{a}{V^2} \right)}} \end{aligned}$$

Ker naloga prepoveduje izražanje s tlakom, moramo na mesto njega vedno vstaviti gornji levi izraz:

$$c_P - c_V = \frac{R}{1 - \frac{2a(V - b)^2}{RTV^3}}$$

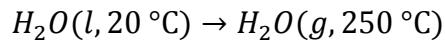
### C) Drugi zakon termodinamike

1) Izračunajte spremembo entropije, če 1 mol N<sub>2</sub> izobarno segrejemo iz 300 na 1000 °C.

$$\overline{c_p} = A + BT + CT^2 \text{ ter } A = 26,983 \text{ } B = 5,91 * 10^{-3} \text{ } C = -3,376 * 10^{-7}$$

$$\begin{aligned}\Delta S &= \int_{T_1}^{T_2} \frac{\overline{c_p}}{T} dT = \int_{T_1}^{T_2} \frac{A}{T} dT + \int_{T_1}^{T_2} BdT + \int_{T_1}^{T_2} CTdT \\ \Delta S &= A \ln \frac{T_2}{T_1} + B(T_2 - T_1) + \frac{C}{2}(T_2^2 - T_1^2) = 36,48 \frac{J}{K}\end{aligned}$$

2) Izračunajte spremembo entropije, entalpije in notranje energije za sledeči proces segrevanja 1 mol vode:



P=1 atm

$$\overline{c_p}(l) = 75,3 \frac{J}{mol K}$$

$$\overline{c_p}(g) = 36,0 \frac{J}{mol K}$$

$$\Delta\bar{H}(izp) = 40668 \frac{J}{mol}$$

$$\begin{aligned}\Delta S &= \int_{T_1}^{T_V} \frac{\overline{c_p}(l)}{T} dT + \frac{\Delta\bar{H}(izp)}{T_V} + \int_{T_V}^{T_2} \frac{\overline{c_p}(g)}{T} dT \\ \Delta S &= \overline{c_p}(l) \ln \frac{T_V}{T_1} + \frac{\Delta\bar{H}(izp)}{T_V} + \overline{c_p}(g) \ln \frac{T_2}{T_V} = 139,3 \frac{J}{K} \\ \Delta H &= \int_{T_1}^{T_V} \overline{c_p}(l) dT + \Delta\bar{H}(izp) + \int_{T_V}^{T_2} \overline{c_p}(g) dT\end{aligned}$$

$$\Delta H = \overline{c_p}(l)(T_V - T_1) + \Delta\bar{H}(izp) + \overline{c_p}(g)(T_2 - T_V) = 52090 J$$

$$H = U + PV \Rightarrow U = H - PV \Rightarrow dU = dH - PdV - VdP$$

$$P = const. \Rightarrow dP = 0 \Rightarrow dU = dH - PdV$$

Predpostavimo idealno obnašanje vodne pare:

$$\Delta U = \Delta H - P\Delta V = \Delta H - P(V(g) - V(l)) \approx \Delta H - PV(g) = \Delta H - RT_2 = 47739 J$$

3) Izračunajte preneseno delo in toploto ter spremembo notranje energije, entalpije in entropije za vsak korak sledečega krožnega procesa enega mola idealnega plina ter za celoten krožni proces.

$$\overline{c_V} = \frac{5}{2} R$$

$$T_1 = 300 \text{ K} \text{ ter } P_1 = 1 \text{ atm}$$

$$\text{izohorno } T_2 = 900 \text{ K}$$

$$\text{izotermno } P_3 = P_1 = 1 \text{ atm}$$

$$\overline{c_P} = \overline{c_V} + R = \frac{7}{2} R$$

### 1→2 izohora

$$\frac{P_1}{T_1} = \frac{P_2}{T_2} \Rightarrow P_2 = \frac{P_1 T_2}{T_1} = 3 \text{ atm}$$

$$V = \text{const} \Rightarrow dV = 0 \Rightarrow dW = -PdV = 0 \Rightarrow W = 0$$

$$dU = dQ \Rightarrow \Delta U = Q = \int_{T_1}^{T_2} \overline{c_V} dT = \overline{c_V} (T_2 - T_1) = 900 R$$

$$\Delta H = \int_{T_1}^{T_2} \overline{c_P} dT = \overline{c_P} (T_2 - T_1) = 1500 R$$

$$\Delta S = \int_{T_1}^{T_2} \frac{\overline{c_V} dT}{T} = \overline{c_V} \ln \frac{T_2}{T_1} = \frac{3}{2} R \ln 3$$

$$2 \rightarrow 3 \text{ izoterna} \Rightarrow T_3 = 900 \Rightarrow T = \text{const} \Rightarrow dT = 0$$

$$dU = \overline{c_V} dT = 0 \Rightarrow \Delta U = 0$$

$$dH = \overline{c_P} dT = 0 \Rightarrow \Delta H = 0$$

$$W = -Q = -RT \ln \frac{V_3}{V_2}$$

$$P_3 V_3 = P_2 V_2 \Rightarrow \frac{V_3}{V_2} = \frac{P_2}{P_3} \Rightarrow W = -Q = -RT_2 \ln \frac{P_2}{P_3} = -900 R \ln 3$$

$$\Delta S = - \int_{P_2}^{P_3} \frac{R dP}{P} = -R \ln \frac{P_3}{P_2} = R \ln 3$$

$$3 \rightarrow 1 \Rightarrow P = \text{const} \Rightarrow dP = 0 \Rightarrow \text{izobara}$$

$$\Delta H = Q = \int_{T_3}^{T_1} \overline{c_P} dT = \overline{c_P} (T_1 - T_3) = -1500 R$$

$$\Delta U = \int_{T_3}^{T_1} \overline{c_V} dT = \overline{c_V} (T_1 - T_3) = -900 R$$

$$W = - \int_{V_3}^{V_1} P_3 dV = -P_3 V_1 + P_3 V_3 = -P_1 V_1 + P_3 V_3$$

$$PV = RT \Rightarrow W = -RT_1 + RT_3 = 600 R$$

$$\Delta S = \int_{T_3}^{T_1} \frac{\bar{c}_P dT}{T} = \bar{c}_P \ln \frac{T_1}{T_3} = -\frac{5}{2} R \ln 3$$

### celokupen krožen proces

$$Q_{\text{S}} = Q_1 + Q_2 + Q_3 = 388,8 R$$

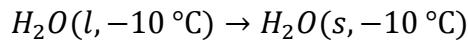
$$W_{\text{S}} = W_1 + W_2 + W_3 = -388,8 R$$

$$\Delta U_{\text{S}} = Q_{\text{S}} + W_{\text{S}} = 0$$

$$\Delta H_{\text{S}} = \Delta H_1 + \Delta H_2 + \Delta H_3 = 0$$

$$\Delta S_{\text{S}} = \Delta S_1 + \Delta S_2 + \Delta S_3 = 0$$

- 4) Izračunajte spremembo entropije ireverzibilnega procesa zmrzovanja enega mol podhlajene vode pri tlaku 1 atm



Kolikšni sta spremembi entropije okolice in celotnega vesolja?

$$\bar{c}_P(l) = 75,3 \frac{J}{mol K}$$

$$\bar{c}_P(s) = 37,2 \frac{J}{mol K}$$

$$\Delta \bar{H}(tal, 0^\circ C) = 6008 \frac{J}{mol}$$

$$\Delta \bar{H}(tal, -10^\circ C) = 5627 \frac{J}{mol}$$

$$\Delta S(\text{proces}) = \int_{T_1}^{T_Z} \frac{\bar{c}_P(l) dT}{T} + \frac{\Delta \bar{H}(tal, 0^\circ C)}{T_Z} + \int_{T_Z}^{T_1} \frac{\bar{c}_P(s) dT}{T}$$

$$\Delta S(\text{proces}) = \bar{c}_P(l) \ln \frac{T_Z}{T_1} + \frac{\Delta \bar{H}(tal, 0^\circ C)}{T_Z} + \bar{c}_P(s) \ln \frac{T_1}{T_Z} = -20,59 \frac{J}{K}$$

$$\Delta S(\text{okolica}) = \frac{\Delta \bar{H}(tal, -10^\circ C)}{T_1} = 21,38 \frac{J}{K}$$

$$\Delta S(\text{vesolja}) = \Delta S(\text{okolica}) + \Delta S(\text{proces}) = 0,79 \frac{J}{K}$$

5) 200 g kositra z začetno temperaturo 100 °C vržemo v adiabatno posodo, v kateri je 100 g vode s temperaturo 25 °C. Izračunajte zmesno temperaturo, spremembo entropije kositra, vode ter adiabatne posode.

$$\overline{c_P}(H_2O) = 75,3 \frac{J}{mol K}$$

$$\overline{c_P}(Sn) = 25,5 \frac{J}{mol K}$$

$$M(Sn)=118,7 \text{ g/mol}$$

$$\frac{m(Sn)}{M(Sn)} \overline{c_P}(Sn)(T(Sn) - T_z) = \frac{m(H_2O)}{M(H_2O)} \overline{c_P}(H_2O)(T_z - T(H_2O))$$

$$T_z = 305,1 K$$

$$\Delta S(Sn) = \int_{T(Sn)}^{T_z} \frac{m(Sn)\overline{c_P}(Sn)}{M(Sn)T} dT = \frac{m(Sn)\overline{c_P}(Sn)}{M(Sn)} \ln \frac{T_z}{T(Sn)} = -8,66 \frac{J}{K}$$

$$\Delta S(H_2O) = \int_{T(H_2O)}^{T_z} \frac{m(H_2O)\overline{c_P}(H_2O)}{M(H_2O)T} dT = \frac{m(H_2O)\overline{c_P}(H_2O)}{M(H_2O)} \ln \frac{T_z}{T(H_2O)} = 9,71 \frac{J}{K}$$

$$\Delta S(posoda) = \Delta S(Sn) + \Delta S(H_2O) = 1,05 \frac{J}{K}$$

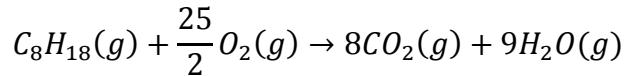
6) Izračunajte entropijo in molsko entropijo mešanja 1 mol O<sub>2</sub> s 3 mol N<sub>2</sub> pri 25 °C ter stalnem tlaku.

$$\Delta S_m = -R \sum_{i=1}^k n_i \ln X_i = -R(n_1 \ln X_1 + n_2 \ln X_2) = 18,7 \frac{J}{K}$$

$$\Delta \overline{S_m} = \frac{\Delta S_m}{n_1 + n_2} = 4,67 \frac{J}{mol K}$$

## D) Gibbsova in Helmholtzova prosta energija

1) Pri temperaturi 298 K ter tlaku 1 bar poteče zgorevanje oktana po sledeči kemijski enačbi:



Izračunajte spremljajoči spremembi Gibbsove in Helmholtzove proste energije.

$$\Delta U = -5109 \text{ kJ}$$

$$\Delta S = 422 \text{ J/K}$$

$$A = U - TS \Rightarrow dA = dU - TdS - SdT$$

$$T = \text{const} \Rightarrow dT = 0 \Rightarrow dA = dU - TdS \Rightarrow \Delta A = \Delta U - T\Delta S = -5235 \text{ kJ}$$

$$G = A + PV \Rightarrow dG = dA + PdV + VdP$$

$$P = \text{const} \Rightarrow dP = 0 \Rightarrow dG = dA + PdV \Rightarrow \Delta G = \Delta A + P\Delta V$$

$$\Delta G = \Delta A + P(V_p - V_r)$$

$$PV = nRT \Rightarrow \Delta G = \Delta A + RT(n_p - n_r) = -5226 \text{ kJ}$$

2) Z vsemi količinami razen s tlakom izrazite notranji tlak mola idealnega oziroma van der Waalsovega plina.

Idealni plin sledi splošni plinski enačbi:

$$PV = nRT; n = 1 \Rightarrow PV = RT \Rightarrow P = \frac{RT}{V}$$

$$\left(\frac{\partial U}{\partial V}\right)_T = T \left(\frac{\partial P}{\partial T}\right)_V - P = T \frac{R}{V} - P = P - P = 0$$

Van der Waalsov plin sledi van der Waalsovi enačbi:

$$\left(P + a \frac{n^2}{V^2}\right)(V - bn) = nRT$$

$$n = 1 \Rightarrow \left(P + \frac{a}{V^2}\right)(V - b) = RT \Rightarrow P = \frac{RT}{V - b} - \frac{a}{V^2}$$

$$\left(\frac{\partial U}{\partial V}\right)_T = T \left(\frac{\partial P}{\partial T}\right)_V - P = T \frac{R}{V - b} - \frac{RT}{V - b} + \frac{a}{V^2} = \frac{a}{V^2}$$

3) Volumen tekoče vode je pri tlaku 1 bar podan z enačbo:

$$V = V_0(1 + aT + bT^2 + cT^3)$$

kjer T predstavlja temperaturo v °C. Poiščite notranji tlak vode ter razliko  $c_p - c_v$  pri 1 °C.

$$a = -6,427 \cdot 10^{-5}$$

$$b = 8,5053 \cdot 10^{-6}$$

$$c = -6,79 \cdot 10^{-8}$$

$$\kappa = 5,18 \cdot 10^{-5} \text{ bar}^{-1}$$

$$\rho_0 = 1 \text{ g/cm}^3$$

$$\left(\frac{\partial U}{\partial V}\right)_T = T \left(\frac{\partial P}{\partial T}\right)_V - P = T \frac{\alpha}{\kappa} - P$$

$$\alpha = \frac{1}{V} \left(\frac{\partial V}{\partial T}\right)_P = \frac{1}{V_0} V_0 (a + 2bT + 3cT^2) = -4,746 \cdot 10^{-5} \text{ K}^{-1}$$

$$\left(\frac{\partial U}{\partial V}\right)_T = T \frac{\alpha}{\kappa} - P = -252 \text{ bar}$$

$$c_p - c_v = \left[ \left(\frac{\partial U}{\partial V}\right)_T + P \right] \left(\frac{\partial V}{\partial T}\right)_P = \left[ \left(\frac{\partial U}{\partial V}\right)_T + P \right] \alpha V_0 = \left[ \left(\frac{\partial U}{\partial V}\right)_T + P \right] \alpha \frac{m}{\rho_0}$$

$$c_p - c_v = \left[ \left(\frac{\partial U}{\partial V}\right)_T + P \right] \alpha \frac{nM}{\rho_0} = 0,0214 \frac{J}{mol \text{ K}}$$

4) Izrazite Joule-Thomsonov koeficient za 1 mol idealnega oziroma van der Waalsovega plina z vsemi količinami razen s tlakom.

Idealni plin sledi splošni plinski enačbi:

$$PV = nRT; n = 1 \Rightarrow PV = RT \Rightarrow V = \frac{RT}{P}; P = \frac{RT}{V}; T = \frac{PV}{R}$$

$$\mu_{JT} = \frac{V(\alpha T - 1)}{c_p}$$

$$\alpha = \frac{1}{V} \left(\frac{\partial V}{\partial T}\right)_P = \frac{1}{V} \frac{R}{P} = \frac{1}{T}$$

$$\mu_{JT} = \frac{V(T^{-1}T - 1)}{c_p} = 0$$

Van der Waalsov plin sledi van der Waalsovi enačbi:

$$\left(P + a \frac{n^2}{V^2}\right)(V - bn) = nRT$$

$$n = 1 \Rightarrow \left(P + \frac{a}{V^2}\right)(V - b) = RT \Rightarrow P = \frac{RT}{V - b} - \frac{a}{V^2}; T = \frac{1}{R} \left(P + \frac{a}{V^2}\right)(V - b)$$

$$\mu_{JT} = \frac{V(\alpha T - 1)}{c_P} = \frac{T \left( \frac{\partial V}{\partial T} \right)_P - V}{c_P} = \frac{1}{c_P} \left[ \frac{T}{\left( \frac{\partial T}{\partial V} \right)_P} - V \right] = \frac{1}{c_P} \left[ \frac{RT}{-\frac{2a(V-b)}{V^3} + \left( P + \frac{a}{V^2} \right)} - V \right]$$

$$\mu_{JT} = \frac{1}{c_P} \left[ \frac{RT}{-\frac{2a(V-b)}{V^3} + \frac{RT}{(V-b)}} - V \right] = \frac{1}{c_P} \frac{2aV(V-b)^2 - RTbV^3}{RTV^3 - 2a(V-b)^2}$$

5) Izrazite odvod  $\left( \frac{\partial P}{\partial V} \right)_S$  z merljivimi količinami. Uporabite dobljeno enačbo za 1 mol idealnega plina.

$$S = f(P, V)$$

$$dS = \left( \frac{\partial S}{\partial P} \right)_V dP + \left( \frac{\partial S}{\partial V} \right)_P dV$$

$$S = const \Rightarrow dS = 0 \Rightarrow 0 = \left( \frac{\partial S}{\partial P} \right)_V (\partial P)_S + \left( \frac{\partial S}{\partial V} \right)_P (\partial V)_S$$

$$0 = \left( \frac{\partial S}{\partial P} \right)_V \left( \frac{\partial P}{\partial V} \right)_S + \left( \frac{\partial S}{\partial V} \right)_P$$

$$-1 = \left( \frac{\partial S}{\partial P} \right)_V \left( \frac{\partial P}{\partial V} \right)_S \left( \frac{\partial V}{\partial S} \right)_P$$

$$\left( \frac{\partial P}{\partial V} \right)_S = -\frac{1}{\left( \frac{\partial S}{\partial P} \right)_V \left( \frac{\partial V}{\partial S} \right)_P} = -\frac{\left( \frac{\partial S}{\partial V} \right)_P}{\left( \frac{\partial S}{\partial P} \right)_V} = -\frac{\left( \frac{\partial S}{\partial T} \right)_P \left( \frac{\partial T}{\partial V} \right)_P}{\left( \frac{\partial S}{\partial T} \right)_V \left( \frac{\partial T}{\partial P} \right)_V} = -\frac{\frac{c_P dT}{T \partial T} \frac{1}{\alpha V}}{\frac{c_V dT}{T \partial T} \frac{\kappa}{\alpha}} = -\frac{\gamma}{V \kappa}$$

Idealni plin sledi splošni plinski enačbi:

$$PV = nRT; n = 1 \Rightarrow PV = RT \Rightarrow V = \frac{RT}{P}; P = \frac{RT}{V}$$

$$\kappa = -\frac{1}{V} \left( \frac{\partial V}{\partial P} \right)_T = \frac{1}{V} \frac{RT}{P^2} = \frac{P}{P^2} = \frac{1}{P}$$

$$\left( \frac{\partial P}{\partial V} \right)_S = -\frac{\gamma}{V \kappa} = -\gamma \frac{P}{V}$$

$$\int \frac{dP}{P} = -\gamma \int \frac{dV}{V}$$

$$\ln P = -\gamma \ln V + const$$

$$\ln P + \gamma \ln V = const$$

$$\ln P V^\gamma = const$$

$$P V^\gamma = konst$$

6) Izrazite odvod  $\left(\frac{\partial H}{\partial U}\right)_T$  z merljivimi količinami. Uporabite dobljeno enačbo za 1 mol idealnega plina.

$$\left(\frac{\partial H}{\partial U}\right)_T = \frac{\left(\frac{\partial H}{\partial V}\right)_T}{\left(\frac{\partial U}{\partial V}\right)_T} = \frac{\left(\frac{\partial H}{\partial P}\right)_T \left(\frac{\partial P}{\partial V}\right)_T}{\left(\frac{\partial U}{\partial V}\right)_T} = \frac{\left[-T \left(\frac{\partial V}{\partial T}\right)_P + V\right] \left(-\frac{1}{\kappa V}\right)}{T \left(\frac{\partial P}{\partial T}\right)_V - P} = \frac{V[\alpha T - 1]}{\kappa V \left(T \frac{\alpha}{\kappa} - P\right)} = \frac{\alpha T - 1}{\alpha T - \kappa P}$$

Idealni plin sledi splošni plinski enačbi:

$$PV = nRT; n = 1 \Rightarrow PV = RT \Rightarrow V = \frac{RT}{P}; P = \frac{RT}{V}; T = \frac{PV}{R}$$

$$\kappa = -\frac{1}{V} \left(\frac{\partial V}{\partial P}\right)_T = \frac{1}{V} \frac{RT}{P^2} = \frac{P}{P^2} = \frac{1}{P}$$

$$\alpha = \frac{1}{V} \left(\frac{\partial V}{\partial T}\right)_P = \frac{1}{V} \frac{R}{P} = \frac{1}{T}$$

$$\left(\frac{\partial H}{\partial U}\right)_T = \frac{\alpha T - 1}{\alpha T - \kappa P} = \frac{T^{-1}T - 1}{T^{-1}T - P^{-1}P} = \frac{0}{0}$$

## E) Odprti sistemi

1) Etilenglikol pri atmosferskem tlaku vre pri 197 °C. Pri kateri temperaturi vre etilenglikol, če je zunanji tlak 0,040 bar?

$$M=62 \text{ g/mol}$$

$$\Delta H_{izp}=799 \text{ J/g}$$

$$\ln \frac{P_2}{P_1} = -\frac{\Delta \bar{H}_{izp}}{R} \left( \frac{1}{T_2} - \frac{1}{T_1} \right)$$

$$\ln \frac{P_2}{P_1} = -\frac{\Delta H_{izp} M}{R} \left( \frac{1}{T_2} - \frac{1}{T_1} \right)$$

$$T_1 = 101,5 \text{ }^{\circ}\text{C}$$

2) Sublimacijska in izparilna krivulja uranovega heksafluorida  $\text{UF}_6$  sledita sledečim enačbam:

$$(s): \log \frac{P}{\text{torr}} = 10,648 - \frac{2559,5}{T}$$

$$(l): \log \frac{P}{\text{torr}} = 7,5396 - \frac{1511,3}{T}$$

Določite tlak in temperaturo trojne točke. Pri kateri temperaturi bi  $\text{UF}_6$  sublimiral, če je zunanji tlak 1 bar?

$$P_3(s) = P_3(l)$$

$$10,648 - \frac{2559,5}{T_3} = 7,5396 - \frac{1511,3}{T_3}$$

$$T_3 = 337,2 \text{ K}$$

$$\log \frac{P_3}{\text{torr}} = 7,5396 - \frac{1511,3}{T_3}$$

$$P_3 = 1142 \text{ torr}$$

$$\log \frac{P_s}{\text{torr}} = 10,648 - \frac{2559,5}{T_s}$$

$$T_s = 329,3 \text{ K}$$

3) Izračunajte temperaturo tališča živega srebra pod površjem Zemlje pri tlaku 100 bar. Pri tlaku 1 bar se živo srebro tali pri -38,87 °C.

$$\frac{\Delta H_{tal}}{m} = 11,63 \frac{J}{g}$$

$$\rho_l = 13,65 * 10^6 \frac{g}{m^3}$$

$$\rho_s = 14,26 * 10^6 \frac{g}{m^3}$$

$$\frac{dP}{dT} = \frac{\Delta H_{tal}}{T \Delta V_{tal}}$$

$$\Delta V_{tal} = V_l - V_s = m \left( \frac{1}{\rho_l} - \frac{1}{\rho_s} \right) = \frac{m(\rho_s - \rho_l)}{\rho_l \rho_s}$$

$$\frac{dP}{dT} = \frac{\Delta H_{tal} \rho_l \rho_s}{T m (\rho_s - \rho_l)}$$

$$\int_{P_0}^P dP = \frac{\Delta H_{tal}}{m} \frac{\rho_l \rho_s}{(\rho_s - \rho_l)} \int_{T_0}^T \frac{dT}{T}$$

$$P - P_0 = \frac{\Delta H_{tal}}{m} \frac{\rho_l \rho_s}{(\rho_s - \rho_l)} \ln \frac{T}{T_0}$$

$$T = -38,25 \text{ } ^\circ\text{C}$$

4) V zaprti posodi z volumnom 10 L imamo 10 g H<sub>2</sub>O. Pri kateri temperaturi, bo 5 g vodne pare v ravnotežju s 5 g tekoče vode?

$$\overline{\Delta H_{izp}} = 40,7 \frac{kJ}{mol}$$

Ker imamo opravka z vodo poznamo temperaturo njenega vrelišča pri normalnem tlaku:

$$T_0 = 100 \text{ } ^\circ\text{C}$$

$$P_0 = 1 \text{ atm}$$

$$\ln \frac{P}{P_0} = - \frac{\overline{\Delta H_{izp}}}{R} \left( \frac{1}{T} - \frac{1}{T_0} \right)$$

Za vodno paro predpostavimo idealno obnašanje:

$$PV = \frac{m_g}{M} RT \implies P = \frac{m_g RT}{MV}$$

$$\ln \frac{m_g RT}{MVP_0} = - \frac{\overline{\Delta H_{izp}}}{R} \left( \frac{1}{T} - \frac{1}{T_0} \right)$$

Temperaturo bomo morali iskati numerično kot ničlo spodnje funkcije:

$$f(T) = \ln \frac{m_g RT}{MVP_0} + \frac{\Delta \overline{H}_{izp}}{RT} - \frac{\Delta \overline{H}_{izp}}{RT_0} = 0$$

Za prvi poskus bomo uporabili temperaturo vrelišča vode pri normalnem tlaku - 100 °C. Nato izdelamo sledečo tabelo:

T [K]	f(T)
373	-0,157
363	0,177

f(T) spremeni predznak in posledično zavzame ničlo med 100 in 90 °C. Posledično lahko temperaturo ocenimo na 95 °C.

5) Vodna ratopina etanola z masnim deležem 3% pri normalnem tlaku 760 torr vre pri 97,11 °C. Kolikšni so parni tlak vode in etanola ter celokupni parni tlak nad vodno raztopino etanola z molskim deležem 2% pri isti temperaturi?

$$P_{H_2O}^0 = 685 \text{ torr}$$

$$X_{et} = \frac{\frac{W_{et}}{M_{et}}}{\frac{W_{et}}{M_{et}} + \frac{W_{H_2O}}{M_{H_2O}}} = 0,012 \Rightarrow X_{H_2O} = 1 - X_{et} = 0,988$$

$$X_{et} K_{et} + X_{H_2O} P_{H_2O}^0 = P$$

$$K_{et} = 6935 \text{ torr}$$

$$X_{et} = 0,02 \Rightarrow X_{H_2O} = 1 - X_{et} = 0,98$$

$$P_{et} = X_{et} K_{et} = 138,7 \text{ torr}$$

$$P_{H_2O} = X_{H_2O} P_{H_2O}^0 = 671,3 \text{ torr}$$

$$P = P_{et} + P_{H_2O} = 810 \text{ torr}$$

6) Idealna vodna raztopina ima pri 100,5 °C tlak vodnih par  $P_A=100,75 \text{ kPa}$ . Izračunajte njenu molalnost.

$$\Delta \overline{H}_{izp} = 40,7 \frac{\text{kJ}}{\text{mol}}$$

Ker imamo opravka z vodo poznamo temperaturo njenega vrelišča pri normalnem tlaku:

$$T_0=100 \text{ } ^\circ\text{C}$$

$$P_0=101,325 \text{ kPa}$$

$$\ln \frac{P_A^0}{P_0} = -\frac{\Delta \overline{H}_{izp}}{R} \left( \frac{1}{T} - \frac{1}{T_o} \right)$$

$$P_A^0 = 103,11 \text{ kPa}$$

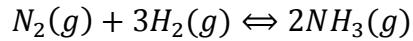
$$X_A = \frac{P_A}{P_A^0} = 0,9771$$

$$X_B = 1 - X_A = 0,0229$$

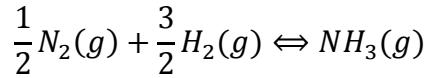
$$m = \frac{n_B}{m_A} = \frac{n_B}{n_A M_A} = \frac{X_B}{X_A M_A} = 1,301 \frac{\text{mol}}{\text{kg}}$$

## F) Kemijsko ravnotežje

1) Pri 400 °C ima reakcija



$K_P^1 = 1,6 \cdot 10^{-4}$ . Kolikšen je  $\Delta G_1^\ominus$ ? Kolikšna sta pri isti temperaturi  $K_P^2$  ter  $\Delta G_2^\ominus$ , če reakcijo preuredimo?



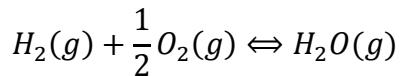
$$K_P^1 = \frac{P_{NH_3}^2}{P_{H_2}^3 P_{N_2}^1}$$

$$\Delta G_1^\ominus = -RT \ln K_P^1 = 48,91 \frac{kJ}{mol}$$

$$K_P^2 = \frac{P_{NH_3}^1}{P_{H_2}^{\frac{3}{2}} P_{N_2}^{\frac{1}{2}}} = \sqrt{K_P^1} = 1,265 \cdot 10^{-2}$$

$$\Delta G_2^\ominus = -RT \ln K_P^2 = 24,46 \frac{kJ}{mol}$$

2) Izračunajte  $K_P$  za sledečo reakcijo pri 25 °C



$$\Delta H_{tv}^\ominus(H_2O) = -241,818 \frac{kJ}{mol}$$

$$S^\ominus(H_2O) = 188,825 \frac{J}{molK}$$

$$S^\ominus(H_2) = 130,684 \frac{J}{molK}$$

$$S^\ominus(O_2) = 205,138 \frac{J}{molK}$$

$$\Delta H_r^\ominus = \Delta H_{tv}^\ominus(H_2O) = -241,818 \frac{kJ}{mol}$$

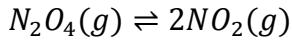
$$\Delta S_r^\ominus = S^\ominus(H_2O) - S^\ominus(H_2) - \frac{1}{2}S^\ominus(O_2) = -44,428 \frac{J}{molK}$$

$$\Delta G_r^\ominus = \Delta H_r^\ominus - T\Delta S_r^\ominus = -228,572 \frac{kJ}{mol}$$

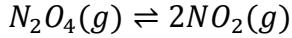
$$\Delta G_r^\ominus = -RT \ln K_P$$

$$K_P = 1,112 \cdot 10^{40}$$

3) Pri temperaturi 318 K ter tlaku 1 bar je stopnja disociacije  $\alpha$  spodnje reakcije 0,38



Določite stopnja disociacije  $\alpha$  ter konstanto ravnotežja  $K_x$  pri tlaku 10 bar.



$$\begin{array}{cccc} t=0 & n_0 & 0 & \Sigma = n_0 \end{array}$$

$$\begin{array}{ccc} t=\infty & n_0(1-\alpha) & 2\alpha n_0 \end{array} \quad \Sigma = n_0(1+\alpha)$$

$$P_i = P X_i$$

$$K_P = \frac{P_{NO_2}^2}{P_{N_2O_4}} = \frac{X_{NO_2}^2 P^2}{X_{N_2O_4} P} = P \frac{\left(\frac{2n_0\alpha}{n_0(1+\alpha)}\right)^2}{\left(\frac{n_0(1-\alpha)}{n_0(1+\alpha)}\right)} = P \frac{4\alpha^2}{1 - \alpha^2} = 0,68$$

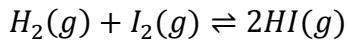
$$K_P = K_X P \Rightarrow K_X = \frac{K_P}{P} = 0,068$$

$$K_X = \frac{4\alpha^2}{1 - \alpha^2}$$

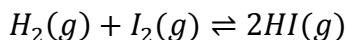
$$K_X = (4 + K_X)\alpha^2$$

$$\alpha = 0,129$$

4) Spodnja reakcija poteka pri konstantnem volumnu in temperaturi

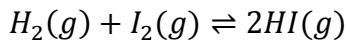


Če dodamo 1 mol  $H_2$  ter 3 mol  $I_2$ , dobimo nekaj  $HI$ . V kolikor dodamo še 2 mol  $H_2$ , pa dobimo dvakrat toliko  $HI$ . Izračunajte  $K_P$ .



$$\begin{array}{cccc} t=0 & 1 & 3 & 0 \end{array}$$

$$\begin{array}{cccc} t=\infty & 1-x/2 & 3-x/2 & x \end{array}$$



$$\begin{array}{cccc} t=0 & 3 & 3 & 0 \end{array}$$

$$\begin{array}{cccc} t=\infty & 3-x & 3-x & 2x \end{array}$$

$$P_i = P X_i$$

$$K_P = \frac{P_{HI}^2}{P_{I_2} P_{H_2}} = \frac{X_{HI}^2 P^2}{X_{I_2} P X_{H_2} P} = \frac{n_{HI}^2 n^2}{n^2 n_{I_2} n_{H_2}}$$

$$K_P^1 = K_P^2$$

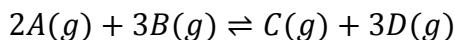
$$\frac{x^2}{\left(1 - \frac{x}{2}\right) \left(3 - \frac{x}{2}\right)} = \frac{4x^2}{(3 - x)^2}$$

$$12 - 8x = 9 - 6x$$

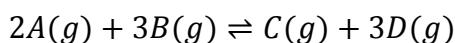
$$x = \frac{3}{2}$$

$$K_p = \frac{4x^2}{(3-x)^2} = 4$$

5) Spodnja reakcija poteka pri temperaturi 25 °C in tlaku 1 bar



Če dodamo 2 mol A, 3 mol B ter 2 mol C, dobimo 2 mol D. Izračunajte ravnotežni konstanti  $K_x$  in  $K_p$  ter  $\Delta G^\ominus$ .



$$t=0 \quad 1 \quad 3 \quad 2 \quad 0$$

$$t=\infty \quad 2/3 \quad 1 \quad 8/3 \quad 2$$

$$\sum n_i = \frac{19}{3}$$

$$P = 1 \text{ bar} \Rightarrow K_p = K_x$$

$$K_p = K_x = \frac{X_C X_D^3}{X_A^2 X_B^3} = \frac{n_C n_D^3 \sum n_i}{n_A^2 n_B^3} = 304$$

$$\Delta G^\ominus = -RT \ln K_p = -14,171 \text{ kJ}$$

6) Pri temperaturi 1000 °C in tlaku 1 bar metan disociira po sledeči reakciji



Konstanta ravnotežja  $K_p$  znaša 128. Izračunajte stopnjo disociacije  $\alpha$  ter ravnotežna molska deleža vodika in metana v plinski mešanici.



$$t=0 \quad n_0 \quad 0 \quad \Sigma = n_0$$

$$t=\infty \quad n_0(1-\alpha) \quad 2\alpha n_0 \quad \Sigma = n_0(1+\alpha)$$

$$K_a = \frac{a_{H_2}^2 a_C}{a_{CH_4}} = \frac{a_{H_2}^2}{a_{CH_4}} = \frac{P_{H_2}^2}{P_{CH_4}} = K_p$$

$$P = 1 \text{ bar} \Rightarrow K_p = K_x$$

$$K_p = K_x = \frac{X_{H_2}^2}{X_{CH_4}} = \frac{\left(\frac{2\alpha n_0}{n_0(1+\alpha)}\right)^2}{\left(\frac{n_0(1-\alpha)}{n_0(1+\alpha)}\right)} = \frac{4\alpha^2}{1-\alpha^2}$$

$$K_p = (4 + K_p)\alpha^2$$

$$\alpha = 0,98$$

$$X_{CH_4}=\frac{1-\alpha}{1+\alpha}=0,01$$

$$X_{H_2}=\frac{2\alpha}{1+\alpha}=0,99$$