



7. Seminar

Sprememba entalpije, sprememba entropije, sprememba proste Gibbsove energije

7. Seminar pri predmetu Kemija 1

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Enačbe

Reakcijska entalpija: $\sum n_{(\text{produkta})} \cdot \Delta H_{t(\text{produkta})} - \sum n_{(\text{reaktanta})} \cdot \Delta H_{t(\text{reaktanta})}$ [kJ/mol]

Entropija sistema: $\sum n_{(\text{produkta})} \cdot \Delta S^{\circ}_{(\text{produkta})} - \sum n_{(\text{reaktanta})} \cdot \Delta S^{\circ}_{(\text{reaktanta})}$ [J/Kmol]

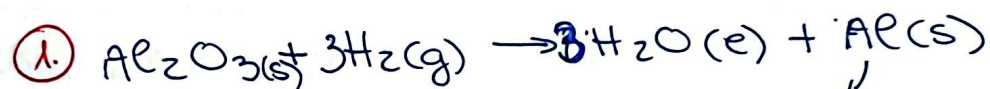
Sprememba entropije: $\Delta S^{\circ}_{(\text{okolice})} = - \frac{\Delta H_{r^{\circ}}}{T}$
 $\Delta S^{\circ}_{(\text{celotna})} = \Delta S^{\circ}_{(\text{okolice})} - \Delta S^{\circ}_{(\text{sistema})}$

Prosta Gibsova entalpija: $\Delta G_{r^{\circ}} = \Delta H_{r^{\circ}} - T\Delta S_r$



Vaja

Koliko je standardna reakcijska entalpija nastanka aluminija iz aluminijevega(III) oksida in vodika?



$$\Delta H_f^\circ(\text{Al}_2\text{O}_3) = -1674,1 \text{ kJ/mol}$$

$$\Delta H_f^\circ(\text{H}_2\text{O}) = -285,5 \text{ kJ/mol}$$

ΔH_f° za elemente je enako $0 \frac{\text{kJ}}{\text{mol}}$

$$\textcircled{2.} \Delta H_r^\circ = \sum \eta(\text{produkta}) \cdot \Delta H_f^\circ(\text{produkta}) - \sum \eta(\text{reaktanta}) \cdot \Delta H_f^\circ(\text{reaktanta})$$

$$\Delta H_r^\circ = 3 \cdot \Delta H_f^\circ(\text{H}_2\text{O}) - 1 \cdot \Delta H_f^\circ(\text{Al}_2\text{O}_3)$$

$$\Delta H_r^\circ = 3 \text{ mol} \left(-285,5 \frac{\text{kJ}}{\text{mol}} \right) - 1 \text{ mol} \left(-1674,1 \frac{\text{kJ}}{\text{mol}} \right)$$

$$\Delta H_r^\circ = (-856,5 - (-1674,1)) \text{ kJ}$$

$$\Delta H_r^\circ = 817,6 \text{ kJ}$$

$$\textcircled{3.} \Delta H_r > 0$$

Endotermna reakcija

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Vaja

Koliko je standardna tvorbeni entalpija etena? Pri gorenju 1 mol etena se sprosti → torej je 1411 kJ energije, tvorbeni entalpiji ogljikovega dioksida in vode pa sta -393 kJ/mol za ogljikov dioksid in -286 kJ/mol za vodo. $\Delta H_r^\circ < 0$

$$\Delta H_r^\circ = -1411 \frac{\text{kJ}}{\text{mol}}$$

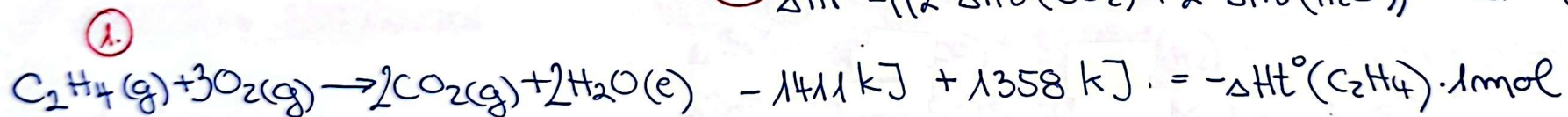
$$\Delta H_f^\circ(\text{CO}_2) = -393 \frac{\text{kJ}}{\text{mol}}$$

$$\Delta H_f^\circ(\text{H}_2\text{O}) = -286 \frac{\text{kJ}}{\text{mol}}$$

$$\textcircled{2} \Delta H_r^\circ = \sum \eta(\text{produkta}) \cdot \Delta H_f^\circ(\text{produkta}) - \sum \eta(\text{reaktanta}) \cdot \Delta H_f^\circ(\text{reaktant})$$

$$\Delta H_r^\circ = (2 \cdot \Delta H_f^\circ(\text{CO}_2) + 2 \cdot \Delta H_f^\circ(\text{H}_2\text{O})) - \Delta H_f^\circ(\text{C}_2\text{H}_4)$$

$$\textcircled{3} \Delta H_r^\circ - ((2 \cdot \Delta H_f^\circ(\text{CO}_2) + 2 \cdot \Delta H_f^\circ(\text{H}_2\text{O}))) = -\Delta H_f^\circ(\text{C}_2\text{H}_4)$$



$$-53 \frac{\text{kJ}}{\text{mol}} = -\Delta H_f^\circ(\text{C}_2\text{H}_4) / (-1)$$

$$\Delta H_f^\circ(\text{C}_2\text{H}_4) = 53 \frac{\text{kJ}}{\text{mol}}$$

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Vaja

Pri reakciji metana in vode je eden od produktov ogljikov . oksid.

- Ali entropija pri nastanku produktov naraste? → Da, saj je št. produktov večje od št. reaktantov
- Izračunajte standardno reakcijsko entalpijo, spremembo entropije okolice in celotno spremembo entropije.
- Ali reakcija poteče spontano?

$$\Delta H_f^\circ(\text{CH}_4) = -74,8 \text{ kJ/mol}$$

$$\Delta H_f^\circ(\text{H}_2\text{O}) = -241,8 \text{ kJ/mol}$$

$$\Delta H_f^\circ(\text{CO}) = -110 \text{ kJ/mol}$$

$$\Delta S_m^\circ(\text{CH}_4) = 186,3 \text{ J/Kmol}$$

$$\Delta S_m^\circ(\text{H}_2\text{O}) = 188,8 \text{ J/Kmol}$$

$$\Delta S_m^\circ(\text{CO}) = 197,7 \text{ J/Kmol}$$

$$\Delta S_m^\circ(\text{H}_2) = 130,7 \text{ J/Kmol}$$

$$\Delta G_r^\circ = \Delta H_r^\circ - T \Delta S_r^\circ$$

$$= 206,6 \frac{\text{kJ}}{\text{mol}} - 298 \text{ K} \cdot 214,7 \frac{\text{J}}{\text{Kmol}}$$

$$= 206,6 \frac{\text{kJ}}{\text{mol}} - 63,9 \frac{\text{kJ}}{\text{mol}} = 142,7 \frac{\text{kJ}}{\text{mol}}$$

reakcija ni spontana

1.

$$\Delta H_r^\circ = \Delta H_f^\circ(\text{CO}) - (\Delta H_f^\circ(\text{CH}_4) + \Delta H_f^\circ(\text{H}_2\text{O}))$$

$$\Delta H_r^\circ = 1 \text{ mol} \cdot (-110 \frac{\text{kJ}}{\text{mol}}) - (1 \text{ mol} \cdot (-74,8 \frac{\text{kJ}}{\text{mol}}) + 1 \text{ mol} \cdot (-241,8 \frac{\text{kJ}}{\text{mol}}))$$

$$\Delta H_r^\circ = -110 \text{ kJ} - (-316,6 \text{ kJ})$$

$$\Delta H_r^\circ = 206,6 \text{ kJ}$$

3.

$$\Delta S_r^\circ = \Delta S_m^\circ(\text{CO}) + 3 \cdot \Delta S_m^\circ(\text{H}_2) - (\Delta S_m^\circ(\text{CH}_4) + \Delta S_m^\circ(\text{H}_2\text{O}))$$

$$\Delta S_r^\circ = ((197,7 + 3 \cdot 130,7) - (186,3 + 188,8)) \frac{\text{J}}{\text{Kmol}}$$

$$\Delta S_r^\circ = (589,8 - 375,1) \frac{\text{J}}{\text{Kmol}}$$

$$\Delta S_r^\circ = +214,7 \frac{\text{J}}{\text{Kmol}}$$

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2.

$$\Delta S_{\text{okolice}}^\circ = - \frac{\Delta H_r^\circ}{T}$$

$$\Delta S_{\text{okolice}}^\circ = - \frac{206,6 \frac{\text{kJ}}{\text{mol}}}{298 \text{ K}} = -0,7 \frac{\text{kJ}}{\text{Kmol}}$$

4.

$$\Delta S_{\text{celotna}}^\circ = \Delta S_{\text{okolice}}^\circ + \Delta S_{\text{stistema}}^\circ$$

$$\Delta S_{\text{celotna}}^\circ = -700 \frac{\text{J}}{\text{Kmol}} + 214,7 \frac{\text{J}}{\text{Kmol}} = -485,3 \frac{\text{J}}{\text{Kmol}} = -485,3 \frac{\text{J}}{\text{Kmol}}$$

Vaja



Pri oksidaciji železa nastane železov(III) oksid. Izračunajte spremembo celotne entropije za to reakcijo, ki poteka pri 25°C. Ali reakcija poteče spontano?

$$\Delta H_f^\circ(\text{Fe}_2\text{O}_3) = -74,8 \text{ kJ/mol}$$

$$\Delta S_m^\circ(\text{Fe}) = 27,3 \text{ J/Kmol}$$

$$\Delta S_m^\circ(\text{O}_2) = 205 \text{ J/Kmol}$$

$$\Delta S_m^\circ(\text{Fe}_2\text{O}_3) = 87,4 \text{ J/Kmol}$$



$$\Delta H_r^\circ = 2 \cdot (-74,8 \frac{\text{kJ}}{\text{mol}}) = -149,6 \text{ kJ}$$

$$\Delta S_r^\circ = 2 \cdot \Delta S_m^\circ(\text{Fe}_2\text{O}_3) - (3 \cdot \Delta S_m^\circ(\text{O}_2) + 4 \cdot \Delta S_m^\circ(\text{Fe}))$$

$$\Delta S_r^\circ = (2 \cdot 87,4 \text{ J/kmol}) - (3 \cdot 205 \text{ J/kmol} + 4 \cdot 27,3 \text{ J/kmol})$$

$$\Delta S_r^\circ = (174,8 - 724,2) \text{ J/kmol}$$

$$\Delta S_r^\circ = -549,2 \text{ J/kmol}$$

$$\Delta G_r^\circ > 0$$

↳ Reakcija ni spontana

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$$\Delta G_r^\circ = \Delta H_r^\circ - T \cdot \Delta S_r^\circ$$

$$\Delta G_r^\circ = -149,6 \frac{\text{kJ}}{\text{mol}} - 298 \text{ K} \cdot (-549,2 \frac{\text{J}}{\text{kmol}})$$

$$\Delta G_r^\circ = -149,6 \frac{\text{kJ}}{\text{mol}} + 163,7 \frac{\text{kJ}}{\text{mol}}$$

$$\Delta G_r^\circ = 14,1 \cdot 10^3 \frac{\text{J}}{\text{mol}}$$