Formelsamling - fysisk kemi

Reversible processer for idealegasser ($w_e = 0$)

	q	w	ΔU	ΔH	ΔS
Isobar $dp = 0$	$n \cdot C_{pm} \cdot \Delta T$	$-p \cdot \Delta V = -n \cdot R \cdot \Delta T$	$n \cdot C_{vm} \cdot \Delta T$	$n \cdot C_{pm} \cdot \Delta T$	$n \cdot R \cdot \ln\left(\frac{T_2}{T_1}\right) + n \cdot C_{vm} \cdot \ln\left(\frac{T_2}{T_1}\right)$
Isochor $dV = 0$	$n \cdot C_{vm} \cdot \Delta T$	0	$n \cdot C_{vm} \cdot \Delta T$	$n \cdot C_{pm} \cdot \Delta T$	$n \cdot C_{vm} \cdot \ln\left(\frac{T_2}{T_1}\right)$
Isoterm $dT = 0$	$n \cdot R \cdot T \cdot \ln\left(\frac{V_2}{V_1}\right)$	$-n \cdot R \cdot T \cdot \ln\left(\frac{V_2}{V_1}\right)$	0 $[= n \cdot C_{vm} \cdot \Delta T]$	0 $[= n \cdot C_{pm} \cdot \Delta T]$	$n \cdot R \cdot \ln\left(\frac{V_2}{V_1}\right)$
Adiabatisk $q = 0$	0	$n \cdot C_{vm} \cdot \Delta T$	$n \cdot C_{vm} \cdot \Delta T$	$n \cdot C_{pm} \cdot \Delta T$	$n \cdot R \cdot \ln\left(\frac{V_2}{V_1}\right) + n \cdot C_{vm} \cdot \ln\left(\frac{T_2}{T_1}\right)$ = 0 hvis rev.

De sidste tre kolonner (H, U og S) gælder også for irreversible processer, da H, U og S er tilstandsfunktioner.

Ud fra idealgasligning kan man skrive mange af formlerne om bl.a.:

$$n \cdot R \cdot T \cdot \ln\left(\frac{V_2}{V_1}\right) = -n \cdot R \cdot T \cdot \ln\left(\frac{p_2}{p_1}\right)$$

Et andet hack: $C_{pm} = C_{vm} + R$

Maxwell-relationer:

For U: $\left(\frac{\partial T}{\partial V}\right)_S = \left(\frac{\partial p}{\partial S}\right)_V$

For H: $\left(\frac{\partial T}{\partial p}\right)_S = \left(\frac{\partial V}{\partial S}\right)_p$

For A: $\left(\frac{\partial p}{\partial T}\right)_V = \left(\frac{\partial S}{\partial V}\right)_T$

For G: $\left(\frac{\partial V}{\partial T}\right)_p = -\left(\frac{\partial S}{\partial p}\right)_T$

De sidste to kan omskrives til $\Delta S = n \cdot R \cdot \ln\left(\frac{V_2}{V_1}\right)$

Tilstand af system: kombination af parametre der beskriver systemet. for os ofte p,V,T
Tilsrandsligning: ligning der beskriver sammenhæng mellem et systemets parametre. F.eks pV=nRT for en idealgas.

$V_m = \frac{M}{\rho}$		
$p = \frac{n \cdot R \cdot T}{V - n \cdot b} - a \cdot \left(\frac{n}{V}\right)^2 = \frac{R \cdot T}{V_m - b} - \frac{a}{V_m^2}$	Van der Waals	Van der Waals (a &b, se tabel 1.6) a= tiltrækkende kræfter mellem molekyler b= volumen per mol molekyler
$a = 3 \cdot p_c \cdot V_c^2,\ b = \frac{1}{3} \cdot V_c$	Van der Waals	a og b udfra kritiske konstanter
$p_r = \frac{p}{p_c},\ T_r = \frac{T}{T_c},\ V_r = \frac{V}{V_c}$		Reduceret variable
$p_r = \frac{8 \cdot T}{3 \cdot V_r - 1} - \frac{3}{V_r^2}$	Van der Waals	Van der Waals med reducerede variable
$a\left(\frac{n}{V}\right)^2 = \pi_T$	Van der Waals	

Entropi (ΔS)

Formel	Gælder når...	Kommentarer
$\Delta S = \int_i^f \frac{\mathrm{d}q_{rev}}{T}$		Def af entropi
$\mathrm{d}S \geq \frac{\mathrm{d}q}{T}$	Generelt	Clausius inequality Dvs. dS ≥ 0 når dq = 0
$n \cdot R \cdot \ln\left(\frac{V_2}{V_1}\right) + n \cdot C_{V,m} \cdot \ln\left(\frac{T_2}{T_1}\right)$	$dp = 0$ eller $q = 0$	
$\Delta S = n \cdot R \cdot \ln\left(\frac{V_2}{V_1}\right) = - n \cdot R \cdot \ln\left(\frac{p_2}{p_1}\right)$	$dT = 0$, ideal	
$\Delta S_{sur} = \frac{q_{sur}}{T_{sur}}$	$dT = 0$ (naturligt for omgivelser), dV=0	
$\Delta S_{sur} = \frac{\Delta H_{sur}}{T_{sur}}$	$dT = 0$, $dp = 0$	
$\Delta S_{sur} = 0$	$q_{sur} = 0$	
$\Delta S_{sur} = 0$	*reversibel*	

$a = \frac{a_0}{Z}$		
$p = \frac{h}{\lambda}$		De Broglie relation p = linear momentum
$p = \frac{h}{\lambda} = \frac{n \cdot h}{2 \cdot L}$	particle-in-a-box	Linear Momentum
$\Psi_n(x) = \sqrt{\frac{2}{L}} \cdot \sin\left(\frac{n \cdot \pi \cdot x}{L}\right)$	particle-in-a-box	n = 1,2… $\left(\frac{2}{L}\right)^{\frac{1}{2}}$ normaliseringskonstant
$E_n = \frac{n^2 \cdot h^2}{8 \cdot m \cdot L^2}$	particle-in-a-box	Energi for ovenstående n = 1,2…
$E_{n+1} - E_n = (2 \cdot n + 1) \cdot \frac{h^2}{8 \cdot m \cdot L^2}$	particle-in-a-box	Energiforskellen mellem lag n og n+1, (→ 0 for L → ∞)
$\lvert\Psi\rvert^2 = \frac{2}{L} \cdot \sin^2\left(\frac{n \cdot \pi \cdot x}{L}\right)$	particle-in-a-box	
$\int \Psi \cdot \Psi_n \, d\tau = 0$	Hvis ortogonale	Ψ_n for forskellige n er altid ortogonale, s. 282
$\tilde{v} = \frac{v}{c} = R \cdot \left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$	Hydrogeniske atomer	Frekvens udsendt $R = \frac{m_e \cdot e^4}{8 \cdot \varepsilon_0^2 \cdot h^3 \cdot c}$ (R_H fås når m_N i stedet for m_e) $\tilde{v}$ = Bølgetallet
$\tilde{v} = Z^2 R_\infty \left\lvert \frac{1}{n_1^2} - \frac{1}{n_2^2} \right\rvert$		Emission af lys $\tilde{v} = \frac{1}{\lambda}$
	Hydrogeniske atomer	Coulomb potentialet