Intermolecular interactions

$$A + B \rightleftharpoons AB$$

DNA strands

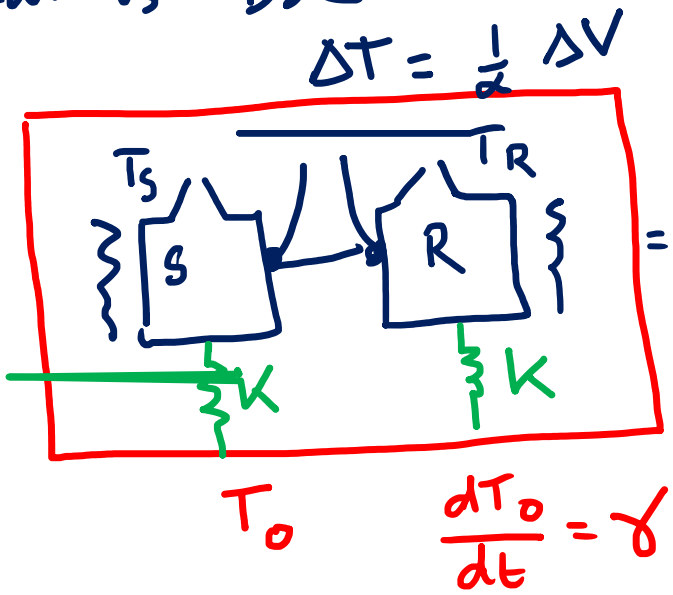
(A) Differential scanning calorimetry

* composition ($n_A = n_B$) is fixed
** T is changed $\gamma = \frac{dT}{dt} = \frac{1.0}{60}$ $K\,s^{-1}$
*** $V_f = 300\,\mu L$

(B) Isothermal titration calorimetry

* T is fixed (25 °C)
** composition is changed
*** $V_s = 1\,mL$ $V_{inj} = 10\,\mu L$ $N = 25$ $t_s = 9000\,s$ $t_i = 600\,s$

(A) what is DSC



R = buffer

S = buffer + A + B

$$P_S = K(T_S - T_0) + C_S \frac{dT_S}{dt}$$

$$P_R = K(T_R - T_0) + C_R \frac{dT_R}{dt}$$

~~stationary~~ regime $\quad \frac{dT_S}{dt} = \frac{dT_R}{dt} = \frac{dT_0}{dt} = \gamma$

$$\Delta P = (P_S - P_R) = K(T_S - T_R) + \Delta C \, \gamma$$

$$\Delta C = (C_S - C_R)$$

① Heat flux $\Delta P = P_R - P_S = 0$

$P_R = 0$ $\quad P_S = 0$

$K\,\Delta T = -\gamma\,\Delta C$

$$\Delta C = -\frac{K}{\gamma}\,\Delta T = -\frac{k}{\gamma}\,\frac{\Delta V}{\alpha}$$

ΔV in μV

all mass is contributing to the signal OK

DNA, proteins $\quad 1/1000 \quad 1\ mg/ml$

② Compensation use ΔP to impose $\Delta T = 0$

$\Delta P = \gamma\,\Delta C$

↓ your signal $\qquad$ ↘ your physical interest

$$\Delta C = \frac{\Delta P\ (\mu V)}{\gamma} = \mu J/K.$$

$A + B \rightleftharpoons AB$ — ~~double stranded~~ helix

↙ ↙

ss stranded

Constant Pressure $\left\{ C_p = \frac{\Delta Q}{\Delta T} = \frac{dQ}{dT} = \frac{\partial H}{\partial T} \right.$

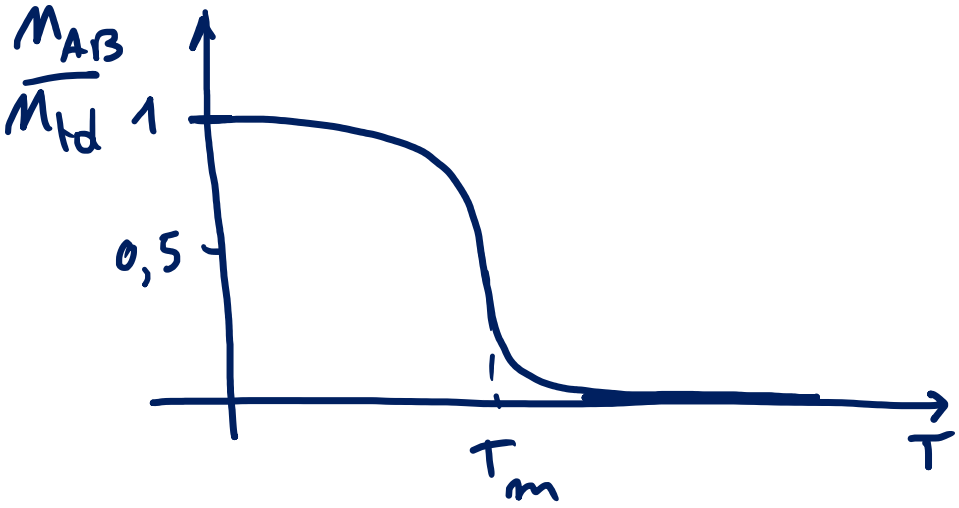
$C_v = \frac{\partial U}{\partial T}$

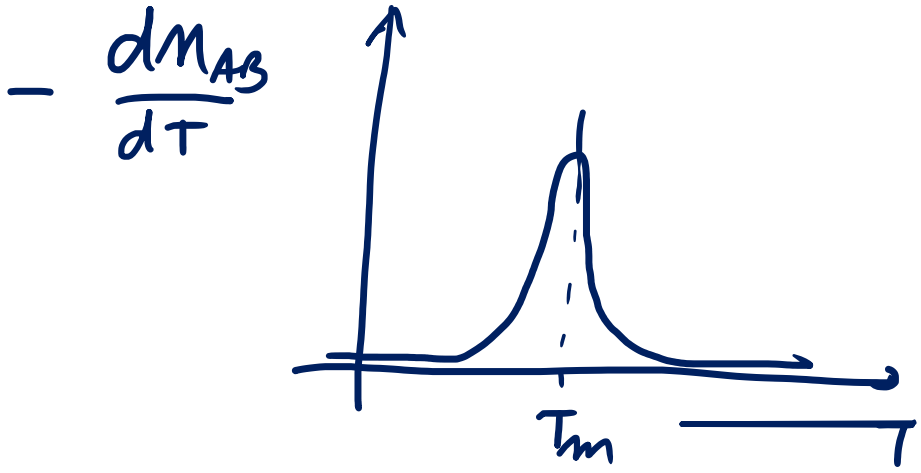
$$H = n_{AB} H_{AB} + n_A H_A + n_B H_B$$

$H_A = H_B = 0$

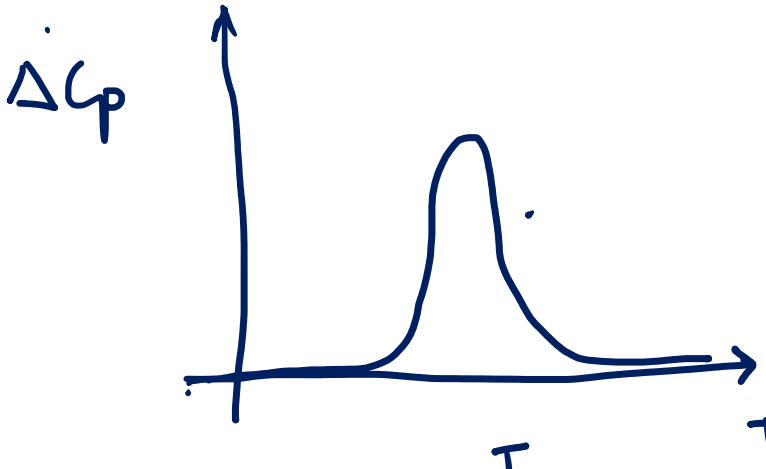
$$\frac{\partial H}{\partial T} = H_{AB} \frac{\partial n_{AB}}{\partial T} + n_{AB} \frac{\partial H_{AB}}{\partial T} \quad (= 0)$$

$$\boxed{C_p = H_{AB} \times \frac{\partial n_{AB}}{\partial T}}$$





$\Delta H_{AB} < 0$

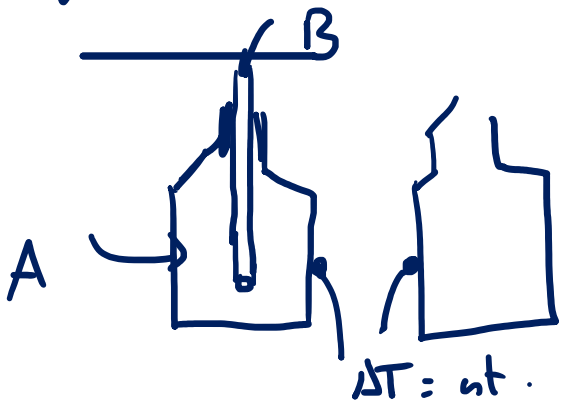


$$\Delta C_p = \Delta H_{AB} \times \frac{\partial n_{AB}}{\partial T}$$

$$\Delta C_p = \frac{\Delta P}{\gamma}$$

$$H_{AB}(F) = \int_{T_0}^{T} \Delta C_p \, dT$$

(B) What is ITC



power to keep ΔT fixed