Oppgave 17a)

Without trial branches, have $P_2 = \frac{1}{4}$ Probability of placing atom 2 such that the full molecule can grow, and $P_3 = \frac{1}{3}$ Probability of placing atom 3 such that it is not rejected.

$$P(k=1) = \frac{1}{4} \cdot \frac{1}{3} = \frac{1}{12} \approx 0,0833$$

17b) Probability of (5,9) being among the trial branches: $P_{tr}(5,9) = 0,5$

Probability of (3,9) being among the trial branches, given that (5,9) is among the trial branches: $P_{tr}((3,9)|(5,9)) = \frac{1}{3}$

Prob. of selecting (5,9) if (3,9) is among branches: $P_{sel}((5,9)|(3,9)) = 0,5$

Prob. of selecting (5,9) if (3,9) is not among branches $= 1 = P_{sel}((5,9)|(\overline{3,9}))$

Probability of selecting (5,9):

$$P_{sel}(5,9) = P_{tr}(5,9)\Big(P_{tr}((3,9)|(5,9))P_{sel}((5,9)|(3,9)) + P_{tr}((\overline{3,9})|(5,9))P_{sel}((5,9)|(\overline{3,9}))\Big)$$

$$P_{sel}(5,9) = 0,5\left(\frac{1}{3} \cdot 0,5 + \frac{2}{3}\right) = \frac{5}{12}$$

For atom 3, (6,9) will be selected if it is among the trial branches.

$$P_{sel}(6,9) = P_{tr}(6,9) = \frac{2}{3}$$

$$P_{gen}(k=2) = \frac{5}{12} \cdot \frac{2}{3} = \frac{5}{18} \approx 0,278$$

$$\frac{P(k=2)}{P(k=1)} = \frac{\frac{5}{18}}{\frac{1}{12}} = \frac{10}{3} \approx 3,33$$

Opg. 17c) Using same notation as in 17b

$$P_{tr}(5,9) = \frac{3}{4}$$

$$P_{tr}((3,9)|(5,9)) = \frac{2}{3}, \quad P_{tr}(\overline{(3,9)}|(5,9)) = \frac{1}{3}$$

$$P_{sel}((5,9)|(3,9)) = \frac{1}{2}$$

$$P_{sel}((5,9)|\overline{(3,9)}) = 1$$

$$P_{sel}(5,9) = P_{tr}(5,9)\left(P_{tr}((3,9)|(5,9))P_{sel}((5,9)|(3,9)) + P_{tr}(\overline{(3,9)}|(5,9))\right)$$

$$P_{sel}(5,9) = \frac{3}{4}\left(\frac{2}{3}\cdot\frac{1}{2} + \frac{1}{3}\right) = \frac{1}{2}$$

$$P_{sel}(6,9) = P_{tr}(6,9) = 1$$

$$P_{sel}(k=3) = \frac{1}{2}$$

$$\frac{P(k=3)}{P(k=1)} = \frac{\frac{1}{2}}{\frac{1}{12}} = 6$$

Oppgave 19)

For only one atom:

Possible States with $y=6$: 10

Possible States with $y=9$: 5

$$\frac{P(y=6)}{P(y=9)} = \frac{10}{5} = \exp\left[\frac{1}{RT}\left(F(9)-F(6)\right)\right]$$

$$F(9)-F(6) = RT\ln\left(\frac{10}{5}\right) = 1728{,}8\ \frac{J}{mol}$$

For 3 atoms:

For $y=6$

x:	1	2	3	4	5	6	7	8	9	10
Possible States:	2	2	6	6	6	2	6	2	2	2

Total possible For $y=6$: 36

For $y=9$

x:	3	4	5	6	7
possible States:	0	2	2	2	3

Total possible For $y=9$: 12

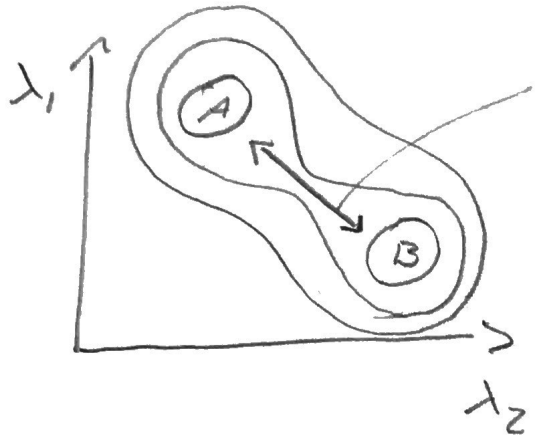
$$\frac{P(y=6)}{P(y=9)} = \frac{36}{12} = \exp\left[\frac{1}{RT}\left(F(9)-F(6)\right)\right]$$

$$F(9)-F(6) = RT\ln\left(\frac{36}{12}\right) = 2{,}7402\ \frac{kJ}{mol}$$

Oppg. 20)

See From the expression For ΔF that $\frac{d}{dT}|\Delta F| > 0$

Oppg. 21)



wish to use this as reaction-coordinate