

## TKJ4215 Statistisk termodynamikk i kjemi og biologi

### Eksamen 27.05.2015, 15.00-19.00

Norges Teknisk-Naturvitenskapelige Universitet

Hjelpemiddelkode A. (Alle trykte og håndskrevne hjelpemidler tillatt. Alle kalkulatorer tillatt.)

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NB: Oppgavene teller ikke like mye. Totalt er 100 poeng fordelt på fire oppgaver. Se parentes etter oppgavenummer for antall poeng per deloppgave.

### Exercise 1 (20, 15, 30, 5)

We have a surface described by a lattice model with  $N$  sites where  $N$  is a large number. We have  $(N - 2)$  A molecules and 2 B molecules. The molecules interact with the energies  $w_{AA}$ ,  $w_{AB}$  and  $w_{BB}$ , respectively. We regard two cases here: case 1) where the two molecules form a dimer, and case 2) where the two molecules are separated from each other (two monomers).

- Derive expressions for Helmholtz free energy for the two cases,  $F_1$  and  $F_2$ .
- Discuss under which conditions case 1 is more favourable than case 2 with respect to temperature and the magnitude of the interaction energies.
- Derive expressions for the vapor pressure for the B molecules. For each case, how does the vapour pressure depend on the interaction energies, and explain the result. Which model do we use for the gas phase and what are the two major approximations in this model?
- Can you based on the results of this exercise give an analogy to the hydrophobic effect?

### Exercise 2 (15)

Which of the following dipole-dipole interaction energies are attractive or repulsive, respectively! Give a (very) brief explanation (no equations allowed)!

- $\rightarrow \rightarrow$
- $\rightarrow \leftarrow$
- $\uparrow \rightarrow$
- $\uparrow \uparrow$
- $\uparrow \downarrow$

### Exercise 3 (10, 5)

a) We can add the surface tension  $\gamma$  to Gibbs free energy in two different ways

$$dG = -SdT + Vdp + \sum_j \mu_j dN_j + \gamma dA$$

$$dG = -SdT + Vdp + \sum_j \mu_j dN_j + Ad\gamma$$

where  $A$  is the area. Explain the distinction between the two equations, and what is the implication for the experimental conditions. For which equation above is

$$\gamma = \left( \frac{\partial G}{\partial A} \right)_{T,p,N}$$

valid. Give a corresponding expression for the other equation.

b) Is the surface tension dominated by an energy or an entropy term? Explain the result in terms of a lattice model.