

**READ THIS FIRST:** You are allowed to use one paper with equations and related notes in the exam. Your equation/note-paper and this exam question paper must be turned in with the answers. You are allowed to use a calculator but clearly show each step of your calculations. Answer all questions.

1.

Macrostate	Energy of level							
	0	1	2	3	4	5	6	7
1	6	0	0	0	0	0	0	1
2	5	1	0	0	0	0	1	0
3	5	2	0	0	0	1	0	0
4	5	0	0	1	1	0	0	0
5	4	2	0	0	0	1	0	0
6	4	1	1	0	1	0	0	0
7	4	1	0	2	0	0	0	0
8	4	0	2	1	0	0	0	0
9	3	3	0	0	1	0	0	0
10	3	2	1	1	0	0	0	0
11	3	1	0	3	0	0	0	0
12	2	4	0	1	0	0	0	0
13	2	3	2	0	0	0	0	0
14	1	5	1	0	0	0	0	0
15	0	7	0	0	0	0	0	0

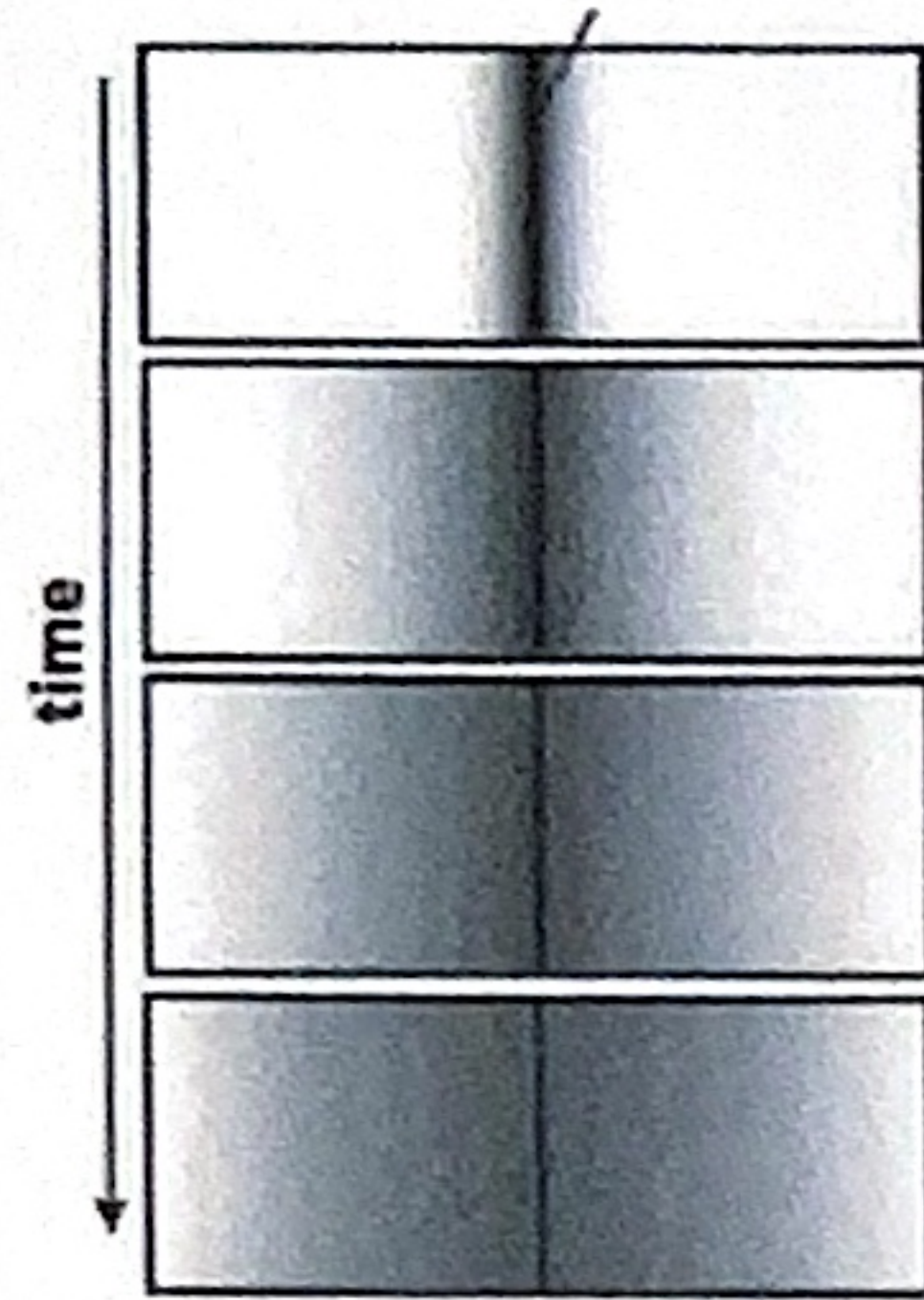
Above is a table of different possibilities (i.e. macrostates) for the occupancy of energy levels in a system with a fixed total energy of 7.

- Which macrostate is the most probable?
- What is the difference in entropy between macrostates 11 and 3?

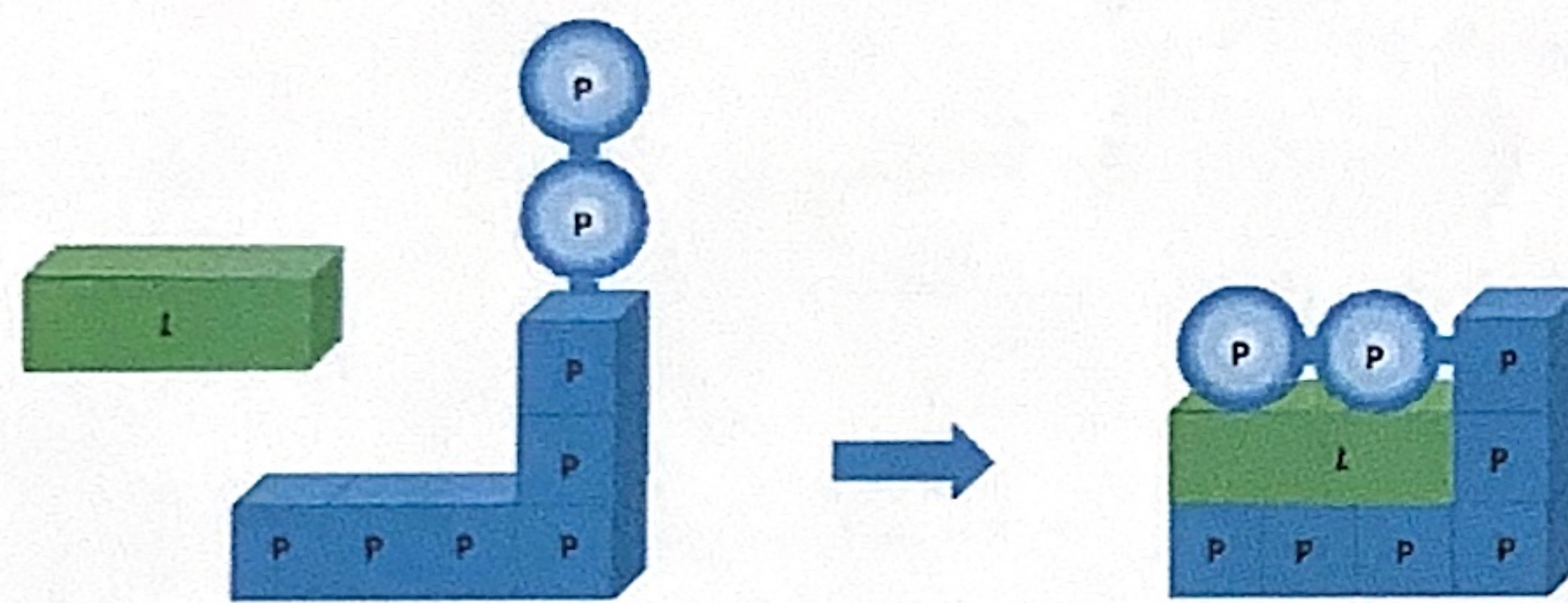
2. The  $\Delta G^\circ$  for ATP hydrolysis is  $-28 \text{ kJmol}^{-1}$  at  $25^\circ\text{C}$  under standard conditions. In the cytoplasm of a bacterium the  $\Delta G$  is kept at  $-50 \text{ kJmol}^{-1}$  for required metabolism to proceed. The bacterium keeps a fixed  $[\text{P}_i]$  at  $15 \text{ mM}$ .

- What is the  $[\text{ATP}] / [\text{ADP}]$  ratio that the bacterium has in its cytoplasm?
- What does the  $[\text{ATP}] / [\text{ADP}]$  ratio go to when the cell dies?
- What is your motivation for your answer in b)

3. Myoglobin protein (MW = 18 kDa) has been applied as a sharp line in a liquid in the middle of a square container. The protein starts to diffuse out towards the ends of the container. The viscosity of the liquid is 1 cP ( $0,01 \text{ g cm}^{-1} \text{ s}^{-1}$ ).



- At a distance of 20 mm from the initial sharp line, how long time will it take until the probability of finding a protein is 50 % of what it is at the initial line? The diffusion coefficient is  $1,11 \cdot 10^{-6} \text{ cm}^2 \text{ s}^{-1}$  at 25 °C.
- How would you describe the meaning of the diffusion coefficient, and in which way would you relate it to the chemical potential?



- In the hypothetical simplified picture above, a ligand (box with L) binds to a protein. A flexible loop closes onto the ligand on binding (circles with P). The rest of the protein is rigid (small boxes with P). The two circles of the flexible loop each have 4 possible orientations. When the loop is closed altogether 6 hydrogen bonds are formed. The change of energy in forming each hydrogen bond in binding is favorable by  $3 \text{ kJmol}^{-1}$ .
  - Calculate the dissociation constant for the binding at 20 °C.
  - Discuss possible contributions to the binding energy that were not taken into account in this simplified model and could be important in a real case?

- The transcription factor **FraJ** binds a poly-A DNA sequence with a  $8 \text{ nM } K_D$  and a poly-G DNA sequence with a  $28 \text{ } \mu\text{M } K_D$ . The concentration of poly-A and poly-G are both  $10 \text{ } \mu\text{M}$ . Mutation of a critical Phe residue to Ala results in a loss of  $21 \text{ kJmol}^{-1}$  in binding free energy for the poly-A sequence, but only a loss of  $3 \text{ kJmol}^{-1}$  on binding to the poly-G sequence. What is the difference in specificity for the poly-A sequence over the poly-G sequence at  $10 \text{ nM}$  concentration of **FraJ** at 300 K?
  - How are the concepts of affinity and specificity related?