

Descriptive tasks (select at least one)

1. Ionic crystals – interactions in ionic crystals and types of their structure.
2. Explain why magnesium, zinc, or aluminium plates are often attached to ship hulls, docks, breakwaters and bridge pillars.
3. The first and second law of thermodynamics and their implications.
4. What is (a) internal conversion; (b) intersystem crossing? What are typical rates of these processes?
5. Compare the equation of state for perfect gas with the van der Waals equation.
6. Types of intermolecular interactions.
7. What are concentration cells and what corresponding systems can be found in nature?
8. The Born-Oppenheimer approximation: its consequences and applications.

Useful constants: $h = 6.626 \cdot 10^{-34} \text{ J}\cdot\text{s}$; $R = 8.314 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$; $k = 1.38 \cdot 10^{-23} \text{ J}\cdot\text{K}^{-1}$; electron mass $= 9.11 \cdot 10^{-31} \text{ kg}$; $c = 2,998 \cdot 10^8 \text{ m/s}$; $1 \text{ eV} = 1,602 \cdot 10^{-19} \text{ J}$; $F = 96485 \text{ C/mol}$

Zadania:

1. Consider the reaction $A(g) \rightleftharpoons 2B(g)$ in equilibrium. Find an expression for α (α is the dissociation degree) as a function of the total pressure of the reaction mixture.

2. A second-order reaction of the type $A + B \rightarrow P$ ($v = k[A][B]$) was carried out in a solution that was initially 0.050 mol L^{-1} in A and 0.080 mol L^{-1} in B. After 1.0 h the concentration of A had fallen to 0.020 mol L^{-1} .
(a) Calculate the rate constant. (b) What was the half-life of the reactants?

3. Which compound should have the higher lattice enthalpy: NaCl or MgO. The respective ionic radii are: $r_{\text{Na}^+} = 116 \text{ pm}$, $r_{\text{Cl}^-} = 167 \text{ pm}$, $r_{\text{Mg}^{2+}} = 86 \text{ pm}$, $r_{\text{O}^{2-}} = 126 \text{ pm}$. Briefly explain your reasoning. What is the length of the unit cell of NaCl?

4. The current of $I = 188 \text{ mA}$ flows through a vessel with a CuSO_4 solution. What time is necessary to cover the cathode area of $A = 25 \text{ cm}^2$ with a copper layer of thickness $l = 0.01 \text{ mm}$? Density of copper, $d = 8.92 \text{ g/cm}^3$, its atomic mass $M = 63.546 \text{ g/mol}$; $F = 96485 \text{ C/mol}$.

5. What is the molar concentration of water in bulk water?

6. Three perfect gases, A, B, and C occupy separate parts of a vessel, with volumes: $V_A = 3 \text{ L}$, $V_B = 5 \text{ L}$, $V_C = 2 \text{ L}$. The whole system is isolated, and the temperature and pressure are the same in all parts of the vessel. After removing the dividing walls, the gases mix. Calculate the entropy change per 1 mole. What is the change in internal energy? $R=8.314 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$.

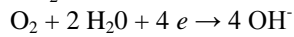
7. 1 mole of N_2 is contained in a 10 L vessel at 300 K. Calculate the pressure and the internal energy, assuming the gas is considered to be perfect. $R=8.314 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$.

8. Consider a molecular crystal consisting of N molecules located in sites of an ideal lattice. Each molecule can assume one of n possible conformations. Energy of the system is independent of conformations. What is the expression for the entropy of the ground state in this system?

9. Consider a one-dimensional classical oscillator with the elastic constant k and mass m . In the initial state the deviation from the equilibrium location is $x=x_0$.

- (a) What was the value of the initial velocity, if in the equilibrium position, $x = 0$, the velocity is v ?
- (b) What is the smallest possible value of the velocity in the equilibrium position ($x = 0$) for a given initial position ($x=x_0$)?

10. The simplest fuel cell is the hydrogen/oxygen galvanic cell, with the following reactions of hydrogen oxidation and oxygen reduction:



The overall reaction is: $2 \text{H}_2 + \text{O}_2 \rightarrow 2 \text{H}_2\text{O}$

ΔG , Gibbs free energy of this reaction is (per 1 mole of H_2O !): $-237200 \text{ J mol}^{-1}$ at 25degree C and $-210300 \text{ J mol}^{-1}$ at 400 degree C. Calculate the potential of this cell under zero-current conditions at both temperatures.

What is the origin of the dependence of the potential on temperature? (Note: in contrast to the Gibbs free energy change (ΔG), the enthalpy change of this reaction (ΔH) depends only weakly on temperature!)

11. Why is the electrolyte in the lead-acid battery (car starting battery) getting diluted during the discharge (and, as a result, its density decreases)?

12. Calculate the activation energy for a reaction of which the rate increases four times when the temperature is raised from 30 to 50 degree C.

13. A piece of metallic cesium was irradiated with light of 700 nm wavelength. Will electrons be ejected from the surface? If so, what will be their kinetic energy? The work function for cesium is 2,14 eV.

14. Normalize the molecular orbital $\psi_s(A) + \lambda\psi_s(B)$ in terms of the parameter λ and the overlap integral S .

15. Provide examples of molecules for which the vibrations will be active (a) simultaneously in the IR and Raman spectra; (b) only in the Raman spectrum; (c) in the IR or in the Raman spectrum.

16. Give examples of molecules of the following symmetries: (a) C_{2v} ; (b) C_{3v} . Describe the corresponding symmetry elements.