



# LIST OF ENTRANCE EXAM QUESTIONS

FOR THE INTERNATIONAL MASTER'S DEGREE PROGRAM

## CHEMISTRY AND ARTIFICIAL INTELLIGENCE

### General chemistry

1. T1. Electronic structure of atoms. Quantum numbers. Order for filling the atomic orbitals for atoms and cations. Shapes of s-, p-, d- atomic orbitals and their dependence on n and m. Nodal planes.
2. Main types of chemical bonds. Valence bond method, hybridization,  $\sigma$ - and  $\pi$ - bonds. The valence shell electron pair repulsion theory and the shape of molecules.
3. Molecular orbitals method (MOM). Overlapping atomic orbitals. The chemical bond in MOM. Energy diagrams of diatomic molecules.
4. Crystal field theory. Tetrahedral and octahedral crystal fields. High and low spin complexes. Crystal field stabilization energy. Ligand strength, spectrochemical series.
5. Crystals and periodicity. Crystal systems. Main packing types: densest packings, AB, AB<sub>2</sub>. Crystal lattice energy and Madelung constant. Dependence of crystal packing on atomic radii ratio exemplified on CsCl, NaCl, ZnS.

### Physical chemistry

6. The first law of thermodynamics. Enthalpy. Hess's Law and its application to the calculation of thermal effects of chemical reactions.
7. The second law of thermodynamics. Reversible and irreversible processes. Entropy. Entropy changes in phase transformations and chemical reactions.
8. Thermodynamic potentials. The equilibrium constant of a chemical reaction. Criteria for the direction and spontaneity of processes.
9. Colligative properties. Dependence of melting and boiling points on the concentration of solute.
10. Thermodynamics of electrolytes. Nernst equation. Impact of complexation and precipitation processes on electrochemical potentials.
11. Phase equilibria. Gibbs' phase rule. Phase diagrams of two component systems. Eutectic point.
12. Kinetics. Reactions of 0th, 1st, and 2nd order. Change of the reaction order during the process. Determining reaction order from experimental data.
13. Elementary step and reaction mechanism. Relationship between reaction mechanism and kinetics. Collision theory. Activated complex theory. Arrhenius equation. Determining activation barrier from experimental data.

### Organic chemistry

14. Alkanes, alkenes, alkynes. Main reactions. Stability of radicals and carbocations. Relationship between structure and regioselectivity of radical substitution and addition. Relationship between structure and regioselectivity of electrophilic substitution.
15. Aromaticity. Hückel's rule. Basic reactions of aromatic compounds. Inductive and mesomeric effects. Regioselectivity of electrophilic substitution.
16. Carbonyl and carboxyl compounds. Condensation reactions. Reactions with alcohols and amines under acidic/basic/neutral conditions. Redox reactions.

## EXAM PREPARATION MATERIALS

### 1 Books

1. Shriver & Atkins Inorganic chemistry, 5th edition.
2. Atkins' physical chemistry, 11th edition.
3. Organic chemistry, J. Clayden, N. Greeves, S. Warren.

### 2 Courses

1. <https://www.youtube.com/playlist?list=PLeo1K3hjS3uvCeTYTeyfeO-rN5r8zn9rw>
2. <https://www.sololearn.com/learning/1094>
3. <https://www.sololearn.com/learning/1073>