General chemistry

1. 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, σ- and π- 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 complex-es. Crystal field stabilization energy. Ligand strength, spectrochemical series.
5. Crystals and periodicity. Crystal systems. Main packing types: densest packings, AB, AB2. Crystal lattice energy and Madelung constant. Dependence of crystal packing on atomic radii ratio exemplified on CsCl, NaCl, ZnS.

General chemistry

6. The first law of thermodynamics. Enthalpy. Hess's Law and its application to the calcula-tion 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. Colligative properties. Dependence of melting and boiling points on the concentration of solute.
9. Thermodynamics of electrolytes. Nernst equation. Impact of complexation and precipita-tion processes on electrochemical potentials.
10. Phase equilibria. Gibbs' phase rule. Phase diagrams of two component systems.
11. Kinetics. Reactions of 0th, 1th, and 2th order. Change of the reaction order during the process. Determining reaction order from experimental data.
12. 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

13. Alkanes, alkenes, alkynes. Main reactions. Stability of radicals and carbocations. Relationship between structure and regioselectivity of radical substitution and addition.
14. Aromaticity. Hückel's rule. Basic reactions of aromatic compounds.
15. 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.

Python programming

17. Data types and structure, lists, tuples, dictionaries, and generators.
18. Math operations in python.
19. Functions in python: syntax, logic and applications.
20. Python loops (loop operators, for, if, while, infinite and nested loops).
21. Working with basic python libraries (numpy, pandas, os, statistics, matplotlib, math, random).
22. Statistical data processing (mean, median, mode, standard deviation, variance, outliers, correlation coefficients).

23. Working with tabular data, dataset characteristics, working with individual columns and rows, removing / adding columns and rows, sorting, filtering and grouping data, merging multiple tables, finding duplicates, applying functions to columns.
24. Data visualization (graphs, histograms, charts, adding header, legend, axes and values captions, text on the graph, building subplots, saving the picture).
25. Data input and output to files of different formats, working with files, adding content to an existing file.

RECOMMENDED LITERATURE

1. Shriver & Atkins Inorganic chemistry, 5th edition.
2. Atkins' physical chemistry, 11th edition.
3. Organic chemistry, J. Clayden, N. Greeves, S. Warren.
4. Downey Allen B. Think Python. Second ed. O'Reilly 2015.