Chemistry MSc Training: Questions for the Final Exam

GROUP A: Common questions including 3 – 4 questions from each general topic taught. This group contains 27 questions. Students admitted for specialized training must answer one question from these. Students without specialization take two questions from this group.

Questions for students with specialization
There are two groups of questions. Anyone who is involved in specialized training must take one question from the corresponding group.

Group B: specialization in analytical chemistry

Group C: specialization in synthetic chemistry

Group A: Common questions
(inorganic, analytical, physical, radio-, organic, bio-, technical chemistry and methods for structural studies)

1. Definition and classification of organometallics. Types of main group organometallics, their binding features and synthetic routes to prepare them. Practical use of organolithium and –magnesium reagents. Isoprene production via organo-aluminium catalysis. Silicon polymers.

2. General characterization of *d*-block organometallics. The most important alkyls, carbonyls, alkenes and η^4-η^8 compounds. Industrial processes with organometallic catalysis: (cross)coupling reactions with Pd-alkyles; the Monsanto process; hydroformylation of alkenes; synthesis of oxo compounds with Pd-alkenes (Wacker-process); homogeneous hydrogenation.

3. Elementary composition and classification of the elements in biological systems. Essential, beneficial and toxic elements and their role in biochemical processes. Coordination chemistry of the most common bioligands including amino acids, peptides, proteins, carbohydrates, nucleotides and porphyrins. Involvement of alkaline and alkaline earth metal ions biological processes: cation distribution and membrane transport processes.

4. Binding, transport and activation of oxygen. The participation of iron and copper in biological oxidation reactions. The structure and properties of iron and copper proteins. Biochemistry of zinc: zinc containing enzymes and zinc finger proteins. The use of inorganic compounds in therapy and diagnosis. Environmental aspects of inorganic substances.

5. Selected fields of nuclear chemistry: thermodynamics of isotopic effects, nuclear reactions. The economical and environmental aspects of nuclear energy production.

6. The definition and types of interface. Adsorption from solutions, formation and structure of charged interfaces, the electric double layer, colloid stability (DLVO). Kinetics of electrode processes, exchange current density, Butler-Volmer equation and its applications. Galvanic cells, batteries and accumulators, fuel cells.

7. Fluid interfaces (G/L, L/L) the concept of surface tension. Laplace-pressure, capillary effects. Biological and biocompatible interfaces. Physico-chemical description and interpretation of biological processes, thermodynamics of living systems, regulation phenomena. Kinetics of enzyme reactions.

8. Efficient methods for the introduction of functional groups and their interconversion, oxidative and reductive transformations, definition and types of synthons. Principle of retrosynthetic approach, retrosynthetic analysis of organic molecules. Characterization of the most important disconnections with examples.

9. General description of the protecting groups and their classifications. Protecting groups of alcohols, phenols and diols, methods for the introduction of the protecting group and cleavage. Protecting groups of the amino, carbonyl and carboxyl groups, their introduction and cleavage.

10. Formation of C–C single and multiple bonds, acid- and base-catalyzed reactions. Synthetic application of enolates and related derivatives. Organometallic reagents and utilization of cross-coupling reactions catalysed by transition metals.

11. Classification and nomenclature of heterocyclic compounds. Preparation and reactivity of three-, four- and five-membered heterocycles with one hetero atom.

12. Five-membered heterocycles with more than one hetero atom. Six-membered heterocycles with one hetero atom and with more than one hetero atom. Six-membered heterocycles.

13. Atomic spectrometry: atomic emission spectrometric methods (ICP-AES), atomic absorption spectrometric methods (graphite furnace AAS), ICP-MS. Theoretical background and applications. Possible interferences. Background correction techniques.

14. Electrochemical methods in analytical chemistry: the principle and realization of the methods,

application fields. Electrogravimetry, coulometry. The fundamentals and instrumentation of polarography. Methods of the polarography. Inverse voltammetry. Cyclic voltammetry.

15. The fundamentals and comparison of chromatographic methods. Realization (instrumentation) and application fields of the chromatographic methods. Ion exchange chromatography. Ion chromatography. Supercritical fluid chromatography. Supercritical fluid extraction.

16. Fundamentals and comparison of electrophoretic methods. Electrophoretic mobility. Realization (instrumentation) and application fields of the electrophoretic methods. Gel electrophoresis and its applications. Detection on gel. Methods of capillary electrophoresis. Electroosmosis.

17. Basic principles of mass spectrometry and main fields of application. Comparison of the different experimental techniques from the point of view of power and applicability. Ion sources and mass analysers used in inorganic chemical applications. Fragmentation reactions and its propriety.

18. Basic principles of NMR spectroscopy and main fields of application. Resonance condition (Larmor equation), chemical shielding, chemical shift, scalar spin-spin coupling, first order spectral analysis (weak coupling). NMR spectral parameters (typical range of ^{1}H and ^{13}C chemical shifts, typical/characteristic values of scalar coupling constants) and their applications in molecular structure determination.

19. Ab initio methods of Quantum chemistry: approximations of Hartree–Fock method, correlation energy and basis sets. Scanning the Potential Energy Hypersurface: determining the stacionary points of the elementary steps of a reaction mechanism.

20. Balance equations. Flows and fluxes. Differential and integral form of balance equations valid for one and two phase unit operations. Transport phenomena. Classification of unit operations.

21. Types and calculation of heat transport. Heat conduction and diffusion. Direct and indirect heat exchange. Temperature-space function of co-current and counter current heat exchangers. Logarithmic mean temperature difference. Types and apparatus of heat exchangers. Equilibrium equations, phase equilibria, equilibrium line and operating line. Definition and determination of the equilibrium unit.

22. Chemical reactors: Classification of reactors based on flow, shape, operation mode, component stream and heat. Operation time, residence time. Concentration-time and concentration-space functions of batch and continuous reactors. Heat balance of a reactor. Selection criteria for a chemical reactor.

23. Crude oil and natural gas: Classification, components. Natural gas and oil processing methods. Motor fuels: The atmospheric and vacuum distillation of crude oil and products. Properties of high-quality gasoline and diesel, octane number, cetane number.

24. Pyrolysis of naphtha: The structure of pyrolyzer furnace, pyrolysis, separation of pyrogas. Thermal cracking, delayed coking, catalytic cracking, hydrocracking, catalytic reforming.

25. Plastics and their application. Commodity plastics: Polyethylene, polypropylene, poly(vinyl-chloride), polystyrene, polyethylene-terephthalate, polyurethanes. Chemical structure, mechanical and thermal properties, chemical resistance.

26. Bioregulation at molecular and cellular level. Hemoglobin function and allosteric regulation. Different strategies in the regulation of enzyme activity: allostery, isoenzymes, reversible covalent modification, limited proteolysis and modulation of enzyme activity with small regulatory proteins. Control by limiting amount of enzyme: regulation of gene expression in prokaryotic and eukaryotic organism at transcriptional level.

27. Sensing the environment in multicellular eukaryotic organisms. The general mechanism of signal-transduction pathways. Interplay between metabolic and signaling pathways. Heterotrimer G protein coupled receptors and their signaling mechanism. Phosphatidylinositol transduction pathway. Signaling by the insulin receptor.

Group B
(analytical chemistry*)*

1. The steps of the chemical analysis. Importance of sampling in analysis. Sampling and sample handling. Planning the sampling, statistical aspects. Sampling procedures for gas, liquid and solid samples. The storage and preservation of the samples. (Baranyai E)

2. Sample pretreatment of organic and inorganic materials for qualitative and quantitative analysis. Decomposing and dissolving the sample. Methods of the atmospheric and high pressure digestions. Kjeldahl digestion. Soxhlet extractor. Solid phase extraction (SPE), solid phase microextraction (SPME), sample enrichments, automated sample pretreatment. (Baranyai E)

3. Characterization and classification of chemical sensors: electrochemical and semiconductor sensors, biosensors, optodes. Attenuated total reflection spectrometry (ATR). Surface plasmon resonance spectrometry (SPR). Labelling analytical methods (ELISA).

4. Methods of continuous flow and kinetic analysis. Flow injection analysis (FIA) and segmented flow analysis. (Flow profiles, instrumentation, on-line sample pretreatment, automated analysis)

5. Modern liquid chromatographic methods módszerek. Ion exchange chromatography. Ion chromatography. Supercritical fluid chromatography. Supercritical fluid extraction.

6. Fundamentals and comparison of electrophoretic methods. Electrophoretic mobility. Realization (instrumentation) and application fields of the electrophoretic methods. Gel electrophoresis and its applications. Detection on gel. Methods of capillary electrophoresis. Electroosmosis. Lab-on-achip.

7. Atomic spectrometry: atomic emission spectrometric methods (ICP-AES), atomic absorption spectrometric methods (graphite furnace AAS), ICP-MS, laser ablation techniques. Theoretical background and applications. Possible interferences. Background correction techniques.

8. Fundamentals and main application fields of mass spectrometry. Ionisation methods, ion sources, analyzers. Comparison of MS instrumentations based on analytical performances and applicability. Hyphenated methods: GC-MS, LC-MS, ICP-MS, CE-MS, tandem MS methods.

9. Electrochemical methods in analytical chemistry (I): the principle and realization of the methods, application fields. Electrogravimetry, coulometry. Karl-Fisher titration with bipotentiometric detection. (Gáspár A)

10. Electrochemical methods in analytical chemistry (II): The fundamentals and instrumentation of polarography and other voltammetric methods. Methods and instrumentation of polarography. Inverse voltammetry. Cyclic voltammetry.

11. Thermal chemical analysis. Instrumentation, methods and main application fields. TG, DTG, DTA, DSC. Derivatography. Thermometric titration. (Gáspár A)

12. Statistical analysis of experimental data. Error and uncertainty in chemical analysis. Confidence intervals. Statistical hypothesis testing (F-test, t-test). Analysis of variance. Linear regression analysis, least squares fitting. Calibration methods: standard addition and internal standards.

13. The quality assurance of analytical methods, accreditation. The history of the quality assurance. ISO systems. Fundamentals and requirements of Good Laboratory Practice (GLP) and Good Manufacturing Practice (GMP). Validation. Analytical performance (validation) parameters.

Group C
(synthetic chemistry)

1. Description of chemical reactions by the perturbation theory. Stereoelectronic effects and their manifestations. Pericyclic reactions: concept and types, synthetic significance, survey and comparison of the methods used for their interpretations.

2. Generation of free radicals. Carbon-centered radicals: stability, reactions and the factors influencing them. Synthetic applications of radical reactions, comparison of ionic and radical reactions.

3. Concept and types of asymmetric transformations. Characterization of the most important starting materials (applied for chiral pool syntheses), their synthetic use for the production of enantiomerically pure target compounds. Substrate-, auxiliary-, reagent- and catalyst-controlled asymmetric synthesis, principles and examples.

4. Principles and examples of kinetic and dynamic kinetic resolution, multiple stereodifferentiation. Introduce some important asymmetric transformations via examples (e.g. alkylation, aldol reaction, oxidation, reduction, organocatalysis, MOC).

5. Parallel syntheses, compound libraries. Solution and solid-phase synthesis techniques, their advantages and disadvantages. Polymer supported substrates, reagents and catalysts. Robotic syntheses. Theory and application of microwave assisted organic synthesis (MAOS). Equipment, techniques of application in organic synthesis. Theory and applications of flow chemistry.

6. Advanced 1D and 2D NMR methods for structural elucidation of organic compounds: selective TOCSY, selective NOE, Watergate, COSY, TOCSY, NOESY, ROESY, HSQC, HMBC.

7. Kinetics and mechanism of cationic and anionic polymerization. Practical applications of the living cationic polymerization.

8. Kinetics and mechanism of radical polymerization (including free radical, NMP and ATRP). Practical applications of the living radical polymerization.

9. Gas chromatographs; types of columns, injectors and detectors. Determination of the chromatographic parameters. Quantitative and qualitative analysis; the GC-MS.)

10. Liquid chromatographs, the HPLC and GPC methods. Types of columns, column technology. Selection of the stationary phase (absorbent). Isocratic and gradient elution. Separation of chiral compounds. Determination of the chromatographic parameters.

11. Configuration of a mass spectrometer, its fundamental components. Principles of the MALDI-TOF MS method and its applications to determine the molecular weight, molecular weight distribution and functionality of synthetic and natural polymers.

12. Atmospheric pressure ionization methods: ESI, APCI and APPI. Online (LC, GPC)-ESI MS. MALDI MS/MS and ESI-MS/MS (PSD, CID) methods and their applications to determine the structure of peptides, oligosaccharides and low molecular weight compounds.