Institute of Chemistry, Department of Physical Chemistry at ELTE
Topics for the Physical Chemistry closing exam (Chemistry MSc)

1. Thermodynamic systems. Laws of classical thermodynamics and their relation to *Callen*'s postulates. The concept of heat, work, energy and entropy. Reversible, irreversible and adiabatic processes. *Carnot* cycle, the efficiency of heat engines.
2. Thermodynamic equilibrium conditions in complex systems. Fundamental equations and equations of state. Energy and entropy representations. Measurable quantities (C_V, C_P, κ_T, κ_S, α): their definition and application. Determination of absolute entropies.
3. The mathematical formalism of thermodynamics. *Euler*'s cyclic chain rule. The *Gibbs–Duhem* equation. *S*, *U*, *H*, *F*, *G* functions and their total derivatives. Conjugated variables. *Maxwell*'s relations.
4. The fundaments of statistical thermodynamics. Describing basic interactions between atoms, ions and molecules (*Coulomb*'s law, *Lennard–Jones* potential, etc.) and the main types of molecular motion (translation, vibration, rotation). Energy distribution and the partition function of canonical and microcanonical ensembles. Molecular partition functions. Thermodynamic potentials and their relation to partition functions. The law of large numbers in thermodynamics.
5. Phase equilibria. Requirements of the equilibrium of phases in single component systems. Gibbs's phase rule. Phase diagrams of single component systems. The *Clapeyron* and *Clausius*–Clapeyron equations. Binary systems and phase diagrams. Eutectic, eutectoid and peritectic phase transitions. Limited miscibility. The critical point. First and second order phase transitions.
6. Ideal and real mixtures. The definition of chemical potential and its dependence on concentration. *Raoult*'s law. Distillation, fugacity, activity. Colligative properties of solutions. Azeotropic mixtures. Isotope effects. The *Joule–Thomson*-effect.
7. Gas laws. The law of corresponding states. The *van der Waals* equation and the virial expansion. The structure of liquids and crystalline solids. Unit cell, *Bravais* lattices. Experimental methods of determining crystalline structure. Glassy and amorphous states, quasicrystals, liquid crystals.
8. Chemical equilibria in reacting systems. The equilibrium constant of homogeneous reactions and its relation to standard reaction potentials under different conditions, expressed with respect to different reference states. Equilibria of heterogeneous reactions. The pressure and temperature dependence of equilibrium constants. The Gibbs–*Helmholtz* equation.
9. Molecular interpretations of chemical reactions: the collision theory and the transition state theory. Reaction rates of elementary reactions: differential forms and simple integral solutions. The quasi-stationarity assumption. Chain reactions and explosions. Catalysis and inhibition. Oscillating reactions and chemical chaos.
10. Transport processes. Heat conduction, diffusion, viscosity, electrolytic conduction. The connection of transport and equilibrium. The continuity equation. The conservation law. Cross-effects.
11. Sensing devices of basic physico-chemical quantities. The principles of calibration; transfer functions. The basics of measurement and control. Temperature and pressure sensors. Methods of concentration measurement at different temporal resolutions. The use of computers in data acquisition and processing.

12. The basics of calorimetry, applications in physical chemistry. Thermal analysis of metallic alloys, experimental determination of phase diagrams in binary systems.
13. Experimental observation of vapour-liquid equilibria of multi-component systems. The characterization of distillers. Phase distribution equilibria. Determination of the heat of evaporation.
14. Methods applicable to determine molar masses. Experimental determination of activities and activity coefficients. Experiments based on colligative properties.
15. Electrodes and electrochemical cells. The electromotive force and its measurement. Determination of thermodynamic reaction parameters by studying the temperature dependence of the electromotive force. Electrochemical power sources.
16. Experimental investigations in thermodynamic systems containing charged particles. Determination of the mean activities and mean activity coefficients in electrolyte solutions. The definition and measurement of *p*H. Methods applied to study limited solubility.
17. Monitoring homogeneous and heterogeneous chemical reactions by different methods; the operating principles of the applied instruments. Determining the kinetic order of chemical reactions. Experimental methods for studying catalytic and autocatalytic reactions.
18. The kinetics of electrode reactions, experimental methods for the investigation of electrode processes. Electrolysis. Conductivity measurements in electrolyte solutions. Ion transport number.
19. Viscosity measurements in gases and liquids. The activation energy of viscous flow and its interpretation. Experimental determination of diffusion coefficients.
20. Surface thermodynamics. Experimental determination of interfacial (surface) tension and the interpretation of the measurements.
21. The principles of quantum mechanics. Physical quantities and their observation, wave functions, expectation values, time-dependent and time-independent *Schrödinger* equations, stationary states, simultaneous determination of observables, *Heisenberg*'s uncertainty principle.
22. The quantum mechanical description of the H atom and many-electron atoms. The *Hamiltonian* and the time-independent Schrödinger equation (energy, eigenfunctions), degeneration, plotting of orbitals, electron density, electron spin, the independent electron approximation, *Pauli*'s principle, *Slater* determinants, orbital energies, the Aufbau principle, electron configuration, notation of atomic states, *Hund*'s rule.
23. The electronic structure of molecules. The Hamiltonian, quantum mechanical treatment of the H_2^+ molecule-ion, orbitals, orbital energies, LCAO–MO approximation. The electronic structure of the H_2 molecule in the VB and MO formalisms. The electron structure of diatomic molecules. The electronic structure of the water molecule in the MO formalism: canonical and localised molecular orbitals.
24. The fundamental aspects of spectroscopy. Factors determining spectra, classification of spectroscopies based on energy ranges and modes of molecular motions involved; the basic interpretation of spectra.
25. Rotational and vibrational spectroscopies. Diatomic molecules in the rigid rotator approximation, energy levels, selection rules. Rotational spectroscopy of many-atom molecules, types of rotors. Applications of rotational spectroscopy.

26. Electron and NMR spectroscopy. The basics of UV–VIS spectroscopy, selection rules, vibrational fine structure, practical applications, the decay of excited states, fluorescence, phosphorescence, the basics of photoionization spectroscopy, ESCA. Magnetic properties of nuclei, the quantum mechanical treatment of nuclear spin, the fundamentals of NMR spectroscopy, qualitative interpretation of spectra, the concept of chemical shift, spin-spin coupling, applications.
27. Excess surface free energy and its consequences. Surface tension, pressure equilibrium between phases separated by a curved boundary, equilibrium vapour pressure above liquid droplets and in cavities, the solubility of small particles.
28. Gibbsian surface thermodynamics. The Gibbs's adsorption equation and its applications. Surface-active and surface-inactive substances. Adsorption isotherms. Equations of state for the adsorption layer.
29. The classical (DLVO) theory of colloidal dispersion stability. Kinetics of coagulation; the effect of electrolyte concentration. Sedimentation, isotherm recrystallization, aggregation.
30. Association colloids, micelle formation, the role of hydrophobic interactions. Solubilisation and mixed micelles.
31. Macromolecular colloids. Polymer solutions. The random coil model. Polymer gels. Polyelectrolytes.
32. Basics of rheology. Flow types and their relation to material properties. Temperature dependence of the rheological behaviour of polymers.