**ITEMIZED LIST**

Physical Chemistry IV: Theoretical Chemistry, advanced level
2017/2018 spring semester

I. *Electronic structure of atoms and molecules*

1. Observations leading to quantum mechanics: particle-wave dualism, properties of electromagnetic field and matter showing quantization (through examples). Postulates of quantum mechanics.
2. Basic concepts of quantum mechanics: physical quantities, their measurements, state function, expectation value, stationary states; simultaneous measurement of two physical quantities; Heisenberg's uncertainty principle; symmetry and the postulate of irreducibility.
3. Example for the analytic solution of Schrödinger equation: particle in the box. Eigenfunctions, eigenvalues, quantization, zero-point energy, degeneracy as consequence of symmetry. The angular momentum operators: commutation relations and eigenvalue problems.
4. The hydrogen atom: principles of solving its Schrödinger equation, eigenvalues, eigenfunctions, quantum numbers. Degeneracy, wave functions and their representations. Electron density, atomic radius, expectation values of physical quantities.
5. The hydrogen atom: magnetic moment, action of magnetic field, Zeeman effect. Phenomenological introduction of spin into quantum mechanics.
6. Basic quantum mechanical description of many-electron systems: Hamilton operator, general form of the wave function and different levels of its approximations; independent particle model (IPM); the Hartree method. Pauli principle (postulate V+2), Slater determinant. A more general form of IPM: the Hartree–Fock (HF) method; interpretation of the results of HF calculations: orbitals, orbital energies, Koopmans principle.
7. Electronic structure of atoms within the independent particle approximation (IPM): orbitals, orbital energies, shells, electron configurations, Aufbau principle, angular momentum of many electron systems. Description and notation of the exact atomic states; Hund's rule, spin-orbit interaction, total angular momentum operator.
8. Electronic structure of molecules: the Born-Oppenheimer approximation; the Hamilton operator. Electronic structure of $H_2^+$. Orbitals, energy as function of the bond distance. Approximate solutions: the LCAO-MO method. Electronic structure of the hydrogen molecule: MO and VB descriptions.
9. Electronic structure of the homonuclear diatomic molecules within the MO approximation: one electron functions, their form and symmetry. Occupation of the orbitals, configuration, bond order, construction of states. Electronic structure of heteronuclear diatomic molecules.
10. Qualitative description of the electronic structure of the water molecule within the MO approximation. Role of symmetry. Canonical and localized orbitals and their relations.
11. Electronic structure of the water molecule within the VB theory. Hybrid orbitals. VB theory and its relation to the Lewis structures.
12. Qualitative description of the electronic structure of many electron molecules within the VB theory: methane, ethene, ethine, ammonia, and the allyl radical.
13. Conjugated π-systems. The Hückel method and its application for ethene, butadiene, and benzene.
14. Electronic structure of transition metal complexes: crystal field theory and ligand field theory.

II. *Theory of structure determination techniques*

1. General overview and history of structure determination techniques. Molecular spectroscopy and quantum chemistry: approximations, energy levels, and selection rules. The electromagnetic spectrum.
2. General characteristics of experimental techniques. Radiation-matter interactions. The laser effect and lasers.
3. Rotational spectroscopy I. Classical mechanics of rotations of polyatomic molecules. Rotational tops.
4. Rotational spectroscopy II. Quantum mechanics of rotations of polyatomic molecules. Energy levels and selection rules.
5. Vibrational spectroscopy I. Basics. Classical description of vibrations of polyatomic molecules. Normal coordinates.
6. Vibrational spectroscopy II. Quantum mechanical description of molecular vibrations. The harmonic linear oscillator.
7. Vibrational spectroscopy III. Symmetry and vibrational spectra. Selection rules. Internal coordinates. Molecular mechanics.
8. Vibrational spectroscopy IV. Vibrational Raman spectroscopy. Selection rules. Depolarization.
9. Electronic spectroscopy I. Basics of visible-ultraviolet (UV-VIS) spectroscopy. Jablonski diagrams. Selection rules.
10. Electronic spectroscopy II. Vibrational fine structure of electronic spectra (Franck–Condon principle). Radiative and non-radiative processes: internal conversion, intersystem crossing, dissociation, predissociation, fluorescence, and phosphorescence.
11. Electronic spectroscopy III. Photoelectron spectroscopy (UPS and XPS).
12. NMR I. General principles of nuclear magnetic resonance spectroscopy. The NMR measurement.
13. NMR II. Chemical shifts and spin-spin couplings. Examples for the interpretation of simple NMR spectra.

The exam starts with a written part (20 minutes, 20 points). At least 50% must be achieved in order to continue the exam. If the written part of the exam is successful, there will be two questions, one from each half of the course.

**Budapest, May 20, 2018** **Attila G. Császár, Péter G. Szalay**