UNIVERSITY OF PANNONIA

COURSE DATASHEET

Semester:	2015/16/1
Course:	Quantum Chemistry I.
Code:	VEMKAKM112K
Responsible department:	Department of General and Inorganic Chemistry
Department code:	MKAK
Responsible instructor:	Dr. György Lendvay

Course objectives:

Acquirement of basic knowledge of general chemistry and chemical calculations.

Course content:

1. Summary of classical mechanics. Motion of atoms in a force field. 2. Élements of molecular mechanics. Quantum effects. 3. Basic principles of quantum mechanics. 6 postulates. Wave functions, operators and their application. 4. Basic mathematical techniques of quantum mechanics: the variational method, perturbation theory and the separation of variables. 5. Quantum mechanics of simple systems I. Particle is a box. 6. Quantum mechanics of simple systems II. The rigid rotor. The principles of rotational spectroscopy. 7. Quantum mechanics of simple systems III. The harmonic oscillator. The principles of vibrational spectroscopy. 8. Calculation of wave functions of atoms I. The hydrogen atom. Written Test I. 9. Calculation of wave functions of atoms II. The He atom. The principles of the Hartree method. 10. The spin of electrons. Magnetic phenomena. The Pauli principle. The wave function for the He atom including spin. The concept of good quantum numbers. Coupling of spin and orbital angular momentum. Basic principles of relativistic effects 11. Antisymmetrization. Slater determinants. The principles of the Hartree-Fock method. 12. Calculation of wave functions of molecules. The Born-Oppenheimer approximation. 13. Calculation of wave functions of molecules. The Born-Oppenheimer approximation. The H2+ ion. ? and ? orbitals. Bonding and antibonding orbitals. The simple MO theory of diatomic molecules. The Hartree-Fock and Valence Bond description of the H2 molecule. The concept of mesomer effect. 14. The Hartree-Fock-Roothaan equations. Convergence-improving techniques (level shifting, quadratic convergence, DIIS). Written Test II. 15. Semiempirical methods. Qualitative pixctures. Orbital interactions.

Requirements, evaluation and grading:

1. Minimum 50% score in 10-minute written tests given at every second week. 2. Minimum 60% score in the two Written Tests. 3. Passing the oral exam at the end of semester (given only if the previous two conditions are fulfilled).

Required and recommended readings:

Kapuy Ede-Török Ferenc: Az atomok és molekulák kvantumelmélete, Akadémiai Kiadó, Budapest, 1975
Mayer István: Kvantumkémia, Budapest, 1980 M. A. Ratner, G.C. Schatz, Introduction to quantum mechanics

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in chemistry, Upper Saddle River, NJ, 2001 J. Simons, J. Nichols: Quantum mechanics in chemistry, Oxford University Press, 1997 Ladik János: Kvantumkémia, Műszaki Könyvkiadó, Budapest, 1960 Póta György: Elméleti Kémia, jegyzet, Debreceni Egyetem, 2000