UNIVERSITY OF PANNONIA

COURSE DATASHEET

Semester:	2015/16/2
Course:	Quantum Chemistry II.
Code:	VEMKAKM212K
Responsible department:	Department of General and Inorganic Chemistry
Department code:	MKAK
Responsible instructor:	Dr. György Lendvay

Course objectives:

Learning the theoretical basis for methods routinely used in quantum chemistry.

Course content:

1. Principles of constructing atomic orbital basis sets. Routinely used AO basis sets. 2. Population analysis, NBO analysis, calculation of bond orders 3. The architecture of quantum chemistry codes and the principles of their operation. 4. Canonical and localized molecular orbitals. The concept of electron correlation. Configuration interaction. 5. Treatment of electron correlation using perturbation theory. 6. Coupled Cluster methods. Multiconfigurtional SCF methods.CAS-SCF. Multireference-CI. Written test I. 7. Density functional theory. The Hohenberg-Kohn snd Kohn-Sham theorems. Exchange and correlation functionals 8. Multilevel ab initio methods. Complete basis extrapolation. 9. Properties of potential surfaces. Geometry optimization. 10. Basic pricniples of calculation of vibrational spectra 11. Basic principles of electronic spectra and their quantum chemical treatment.

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, Quantum mechanics in chemistry, Wiley, 1998 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