THEORY OF CHEMICAL REACTIVITY.

B.Nagy Ottó D.Sc.

Retired Professor, Catholic University of Louvain (UCL), Louvain-la-Neuve, Belgium.

Former Head of the Physical Organic Chemistry Laboratory.

The aim of the course is to present simple theoretical methods for the interpretation of chemical reactivity, leading to understanding and predicting possible outcomes of a given reaction. The approach will be essentially practical that will allow the students to apply by themselves the presented methods to actual reactivity problems.

The following topics will be discussed: basic principles of quantum theory; molecular orbitals (LCAO-MO); the two-center problem; ab initio and density functional methods; the HÜCKEL method by variation (HMO) and perturbation (PMO) approaches; general perturbation theory; population analysis; free-electron (FEMO), non-bonding orbital (NBMO) and linear combination of molecular orbitals (LCMO) methods; aromaticity; applications of HMO method; reactivity indices; the localization method; FUKUI frontier orbital (FMO) approach; substituent effects and transition state properties; systematic application of intra- and inter-molecular perturbation theory to chemical reactions; linear free energy relationships (LFER); soft and hard acids and bases(SHAB) and the density functional theory (DFT); orbital interactions in molecules; non-classical ions, anomeric effect, cis-trans isomerization; the rôle of symmetry in chemical reactions; potential energy surfaces(PES).

Selected reference sources:

-Quantum Chemistry, I.N. Levine, Prentice Hall, New Jersey.

-Density-Functional Theory of Atoms and Molecules, R.G. Parr, W. Yang, Oxford University Press, New York.

-Podstawy i Metody Chemii Kwantowej, R.F. Nalewajski, PWN, Warszawa.

-Molecular Orbital Theory for Organic Chemists, A. Streitwieser, John Wiley, New York.

-Das HMO-Modell und seine Anwendung, I-III, E.Heilbronner, H.Bock, Verlag Chemie, Weinheim.

-Frontier Orbitals and Organic Chemical Reactions, I. Fleming, John Wiley, London.

-The PMO Theory of Organic Chemistry, M.J.S. Dewar, R.C. Dougherty, Plenum/Rosetta, New York.

-Chemical Applications of Group Theory, F.A. Cotton, John Wiley, New York.

Termin	Dzień tygodnia	Godzina	Miejsce
20.03.2017	Poniedziałek	12.15 – 15.00	Minicentrum Konferencyjne (Luwr)
21.03.2017	Wtorek	12.15 – 15.00	Minicentrum Konferencyjne (Luwr)
22.03.2017	Środa	12.15 – 15.00	Minicentrum Konferencyjne (Luwr)
23.03.2017	Czwartek	12.15 – 15.00	Minicentrum Konferencyjne (Luwr)
24.03.2017	Piątek	12.15 – 15.00	Minicentrum Konferencyjne (Luwr)