UNIVERSITY OF PANNONIA

COURSE DATASHEET

Semester:	2016/17/1
Course:	Stereochemistry of organic compounds
Code:	VEMKOK5112S
Responsible department:	Department of Organic Chemistry
Department code:	MKOK
Responsible instructor:	Gergely Farkas

Course objectives:

Educational Objectives: By the knowledge of basic principle of stereochemistry to gain reliable rationalisations of many aspects of chemical reactions.

Course content:

Contents: Week 1. Static stereochemistry, configuration and chirality. 2. Molecular geometry, molecular symmetry. 3. Symmetry in simple carbon compounds, classification of molecules according to their symmetry. 4. Stereoisomers and chirality, molecular chirality. 5. Molecules containing more than one centre of asymmetry. 6. The experimental determination of configuration. 7. Principle relating to the separation of enantiomers, conformation of carbon compounds. 8. Dynamic stereochemistry. Methods of dynamic stereochemistry. Intramolecular symmetry relations between the groups of the same structure and position. Topicity. Molecular symmetry and NMR spectroscopy. 9. The kinetics of configurational and conformational change, racemization and epimerization, configurational inversion. 10. Hindered rotation about single and double bonds, conformational equilibrium in ring systems. Ring inversion. 11. Applied stereochemistry, Reactivity and molecular symmetry. 12. Transformations involving structurally identical groups and molecular faces. 13. Formation of stereoisomers, reactivity of enantiomers, diastereomers. Configuration, conformation and reactivity. 14. Determination of enantiomeric purity. 15. Stereoisomers of monotonic polymers. Stereoisomers of some inorganic complexes.

Requirements, evaluation and grading:

Examination Requirements and Questions: Historical background (Malus, Biot, Arago, Pasteur, Kekule, van't Hoff, Le Bel, Hassel, Mislow, Chan-Ingold-Prelog). Important concepts in stereochemistry: three dimensional aspects of chemistry, art and symmetry, nature and symmetry, biological properties (taste, flavour and structure), structure and reactivity. Geometrical parameters of molecules: the van der Waals' radius, the bond length, the bond angle, dihedral angle. Molecular symmetry, elements of symmetry (plane and axis of symmetry, rotation- reflection symmetry). Symmetry in simple carbon compounds: one-, two-, three- and four-coordinate carbon compounds.. Classification of molecules according to their symmetry. Schönfliess point groups. Point groups relevant to chemistry and symmetry. Chiral point groups (Cn, Dn): C1, C2, C3, C6; Dn dihedral point group (n-bladed propellers): D2, D3, D4. Achiral point groups: Cs, Sn, Cnv, Cnh, Dnd, Td. Cs: Sn: S2 S4, S6. Cnv: C2v, C3v, C4v. Cnh: C2h, C3h. Dnd: D2d, D3d. Dnh: D2h, D3h,, D6h. Td. Classification of molecules by their symmetry. Significance of chiral molecules: enantiomers, diastereomers, the sequence rules relating to the chirality of centres (Fischer-projection, the convention of Cahn-Ingold-Prelog), chirality of

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central, axial, planar, or helical. Molecules containing more than one centre of asymmetry (conformation and statistical symmetry of tartaric acids). Chiral and achiral conformations of meso tartaric acid. Pseudo-chirality (centrum, plane, axis). Pseudo-asymmetry and its practical application for the determination of enantiomeric excess using achiral reagents. The experimental determination of the absolute and relative configuration. Chiroptical methods: optical rotary dispersion (ORD) and circular dichroism (CD). Interaction of polarised light with chiral and achiral media. Positive and negative Cotton effect. Chiral chromophores. Relation between configuration and Cotton effect. Application of octant rule for ketones. Chiroptical properties of ketones. Methods for the determination of enantiomeric purity: polarimetry, basic principle of glc and HPLC separation, NMR spektroscopic methods (CDA, chiral solvating agent; chiral lanthanide shift reagent (CLSR), achiral reagents. The kinetics of conformational and configurational change. Hindered rotation about single bond and double bond. Conformational equilibrium in ring systems. Reactivity of stereoisomers: the relative reactivity of enantiomers and diastereomers.

Required and recommended readings:

Felhasznált tankönyvek: 1. Nógrádi, M.: Bevezetés a sztereokémiába, Muszaki Könyvkiadó, Budapest (1975). 2. Nógrádi, M.: Stereochemistry, Basic Concepts and Application, Akadémiai Kiadó, Budapest (1981). 3. Eliel, E. L., Willen, S. H.: Stereochemistry of Organic Compounds, John Wiley and Sons, Inc., New York Budapest (1994). 4. Juaristi, E.: Introduction to Stereochemistry and Conformational Analysis, John Wiley and Sons, Inc., New York (1991). 5. Nógrádi, M.: Stereoselective Synthesis, VCH, Weinheim (1995). 6. Aitken, R. A., Kilényi, S. N.: Asymmetric Synthesis, Blackie Academic and Proffessional, London, (1994). 7. Alworth, W. L.: Stereochemistry and its Application in Biochemistry, Wiley Interscience, New York (1972). 8. Simonyi, M.: Problems and Wonders of Chiral Molecules, Akadémiai Kiadó, Budapest (1990). 9. Collins, A. N., Sheldrake, G. N., Crosby, J.: Chirality in Industry. The Commercial Manufacture and Application of Optically Active Compounds, John Wiley and Sons, Inc., New York (1992). 10. Potapov, V. M.: Stereochemistry, MIR Publishers, Moscow (1979). 11. Allenmark, S.: Chromatographic Enantioseparation, Ellis Horwood, New York (1991). 2. Sheldon, R. A.: Chirotechnology, Marcel Dekker, Inc., New York (1993).