

# Popis předmětu

<b>Zkratka předmětu:</b>	UCH/952	<b>Strana:</b>	1 / 2
<b>Název předmětu:</b>	Mol. Environ. & Bio-org. Mol. Structure		
<b>Akademický rok:</b>	2012/2013	<b>Tisknuto</b>	20.03.2013 08:24

<b>Pracoviště / Zkratka</b>	UCH / 952	<b>Akademický rok</b>	2012/2013
<b>Název</b>	Mol. Environ. & Bio-org. Mol. Structure	<b>Způsob zakončení</b>	Zkouška
<b>Název dlouhý</b>	Molecular Environment and Bio-organic Molecular Structure		
<b>Akreditováno/Kredit</b>	Ano, 5 Kred.	<b>Forma zkoušky</b>	Kombinovaná
<b>Rozsah hodin</b>	Přednáška 1 [TYD/SEM]		
<b>Obs/max</b>	Statut A      Statut B      Statut C	<b>Zápočet před</b>	ANO
<b>Letní semestr</b>	0 / -      0 / -      3 / -	<b>Počítán do průměru</b>	ANO
<b>Zimní semestr</b>	0 / -      0 / -      0 / -	<b>Min. (B+C) studentů</b>	nestanoveno
<b>Vyučovací jazyk</b>	Angličtina	<b>Opakovaný zápis</b>	NE
<b>Nahrazovaný</b>		<b>Vyučovaný semestr</b>	Letní semestr
<b>Vyloučené předměty</b>			

## Cíle předmětu (anotace):

Special Topics in Molecular Environment and Bio-organic Molecular Structure.

Lecture 1- The language of structural chemistry and its symmetry basis

Lecture 2- Symmetry operations and site permutations

Lecture 3- New system to classify isomers based upon isometry: homomers, enantiomers, diastereomers, and constitutional isomers

Lecture 4- Stereogenic elements: tetrahedral atoms, helicity

Lecture 5- All Sohncke space groups preserve the handedness of the exchanged molecules

Lecture 6- Unequal population distribution of the 230 space groups

Lecture 7- Chiral apple halves and helical stereochemistry

Lecture 8- Chiral apple halves and helical stereochemistry II

Lecture 9- Symmetry in NMR spectroscopy

Lecture 10- Chiral Recognition via Helical Sense and Phase in a crystalline supramolecular array of intereshed triple-helices

Lecture 11- What something is depends on where you put it

Lecture 12- What something is depends on where you put it II

Lecture 13- Dynamic stereochemistry, permutations, correlated motion and DNMR

Lecture 14- Diaryl-X propellers ground state geometry

## Požadavky na studenta

## Obsah

Contents of selected lectures:

Lecture 1- The language of structural chemistry and its symmetry basis:

Isometry and symmetry. The eight symmetry operations. Man's genetic predisposition to symmetry. Neanderthal stone axe heads. Pseudosymmetry is a continuum of distortion from symmetry. Symmetry and the Golden Ratio. Symmetry in beauty- an interpretation of physical health. Mankind's fascination of high symmetry objects- high symmetry stone carvings by the Celts, 4000 years ago. The Convex Platonic Solids. Almost all perceived symmetry is approximate symmetry. DaVinci's vitruvian man painting and the golden ratio. Internal versus external symmetry comparisons. Symmetry elements, symmetry operations, special/general positions. Occupancy of special positions of symmetry in crystals.

Lecture 2- Symmetry operations and site permutations. Elementary Group Theory and symmetry equivalence. Point groups and space groups. Molecular dissymmetry and Chirality (handedness). Chirality is a continuum of distortion from achirality. Chiral is not an equivalent term to asymmetric. The I-symmetry icosahedral chiral protein viral capsid of the retrovirus. Molecular structure. Constitution. Bonding parameters. Difference between dihedral and torsion angles.

Lecture 7- Chiral apple halves and helical stereochemistry: Cinquini and Cozzi elegantly demonstrated the

bisection of an achiral molecule into two homochiral halves. The stereochemical outcome of these chemical reactions was linked to the parlor trick known as 'la coupe du roi'. La coupe du roi bisection removes all symmetry operations of the second kind. Coupe du roi cutting steps. The bisection product is a D<sub>2</sub>-symmetry chiral ensemble. This ensemble consists of two C<sub>2</sub>-axis related homochiral halves nestled together so that they may be readily separated. This operation may be utilized to polysection objects having C<sub>2v</sub> or D<sub>2h</sub> symmetry. Achiral objects are desymmetrized by la coupe du roi into C<sub>n</sub> or D<sub>n</sub> symmetry chiral ensembles of n-segments, where each segment is homotopically related to the others via a mutual C<sub>n</sub>-axis. When translated one repeat unit either upwards or downwards, the 2 coupe du roi halves mutually complete one full turn of a single right-handed (P)-41-helix or left-handed (M) 43-helix. An in-depth view of screw displacement (screw-rotation). Nm right-handed screw displacement (P)- n1-helices. Nm left-handed screw displacement (M)- nn-1-helices. Mislow, Anet, and coworkers reported the 'inverse coupe du roi' that is based upon chiral discrimination.

Lecture 13- Dynamic stereochemistry, permutations, correlated motion and DNMR: Correlated motion in bis(9-triptycyl)-X nanomachines. Phase isomers. Mechanics of linear versus cyclic gear trains. Graph Theory hexagonal Caley diagram cogwheeling circuit and permutational isomers of stereochemically labeled di(9-triptycyl)-ether (sulfide, or methane). Enantiomers of the cogwheeling circuit are on another hexagonal graph. Phase isomers can not interconvert by free cogwheeling motion. If the ca. 1 kcal energy barrier for cogwheeling motion is so low then how do you describe the molecule's structure with only one picture? Residual characteristics of a group and residual isomerism. Residual enantiomers and residual diastereomers. Lecture 14- Diaryl-X propellers ground state geometry. Aromatic ring geometry in helicity change transition states. 0-,1-, and 2-ring flip transition-state site exchange. Correlated motion in diaryl-X propellers. Binary numerical descriptors for permutational isomers. Graph Theory square Caley diagram cogwheeling circuit and permutational isomers of stereochemically labeled diaryl-X propellers (ether, sulfide, methane). ). None of the 1-ring flip structures in a cogwheeling circuit is the enantiomer of the other.

## Předpoklady - další informace k podmíněnosti

## Získané způsobilosti

## Garanti a vyučující

- **Garanti:** prof. Robert Glaser
- **Přednášející:** prof. Robert Glaser

## Literatura

## Vyučovací metody

## Hodnotící metody

## Předmět je zařazen do studijních programů: