Concepts of Molecular Chemistry I (iMOS)

Module	Credits	Workload	Term	Frequency	Duration
5 RC	5 CP	150 h	1. Sem.	WS	1 Semester
Courses			**Contact hours**	**Self-Study**	**Group size**
a) Lecture b) Exercises			a) 2 SWS / 30 h b) 1 SWS / 14 h	105 h	30 Students

Prerequisites

Learning outcomes

Students acquire advanced knowledge on the theory and techniques of the basic concepts of physical organic chemistry such as bond models, thermochemistry, and the theoretical evaluation of properties of experimental interest, in particular the theory of potential energy reaction surfaces. The main focus lies on the interplay between theoretical and experimental methods.

Students learn to read and understand advanced selected scientific publications in the topic of physical organic chemistry, how to summarize the publication in an abstract, and to present the essentials of the publication in an oral presentation using presentation software (15 min + 5 min discussion).

Content

- The covalent chemical bond (properties, experimental methods)
- The non-covalent chemical bond (van der Waals complexes, hydrogen bonds, supramolecular chemistry, peptides)
- Thermochemistry (properties, Benson's additivity rules)
- Potential energy surfaces (internal coordinates, Born Oppenheimer approximation, stationary points, reaction coordinates, Marcus theory, Curtin Hammett principle, More O'Ferral-Jencks diagrams, reactivity and selectivity, tunneling)
- Force field calculations (MM2)
- Linear free energy relations
- Experimental techniques (matrix isolation)

Teaching methods

Lecture, seminar based teaching with active participation of the student

Mode of assessment

30 min end-of-term oral exam or 2-hour end-of-term written exam

Requirement for the award of credit points

Successful oral presentation, passing the exam

Module applicability

M.Sc iMOS Required Course; cross-posted M.Sc. Chemistry as Concepts of Molecular Chemistry I: Physical Organic Chemistry

Weight of the mark for the final score

According to CPs

Module coordinator and lecturer(s): W. Sander

Further information