MSc Chemistry Module Guide

pursuant to

the Examination Regulations of

September 8, 2020

Content

Abbreviations

FMNS	Faculty of Mathematics and Natural Sciences
L	Lecture
E	Exercise
S	Seminar
LC	Lab course
CP	Credit points
ECTS	European Credit Transfer System
SLT	Self-learning time
en.	English

Module Overview

Program starting in the winter semester

Semester	Module	Module	Module	Module	Total
1. Sem.	**MCh 20 1.1** *Advanced Inorganic Molecular and Solid State Chemistry* L, S 10 CP	**MCh 20 1.2** *Organic Molecules and Materials* L, S 10 CP	**MCh 20 1.3** *Advanced Physical Chemistry* L, E 5 CP	**MCh 20 1.4** *Quantum Chemistry* L, E 5 CP	**30 CP**
2. Sem.	**MCh 20 2** *Analytical Methods for Condensed Matter* L, S 10 CP	**MCh WP*** *Elective modules* 20 CP			**30 CP**
3. Sem.	**MCh WP*** *Elective modules* 20 CP	**MCh 20 3** *Focusing Laboratory Course* 10 CP			**30 CP**
4. Sem.	**MCh 20 4** *Master of Science Thesis* 30 CP				**30 CP**

* A total of 4 elective modules must be completed.

WP-modules in the winter term: WP 8, WP 9, WP 10, WP 11, WP 12, WP 13, WP 14, WP 15, WP 16 (duration: 2 semesters)

WP-modules in the summer term: WP 1, WP 2, WP 4, WP 5, WP 6, WP7, WP 17

Program starting in the summer semester

Semester	Modules				Total
1. Sem.	**MCh 20 2** *Analytical Methods for Condensed Matter* L, S — 10 CP	**MCh 20 1.2** *Organic Molecules and Materials* L, S — 10 CP	**MCh 20 1.3** *Advanced Physical Chemistry* L, E — 5 CP	**MCh 20 1.4** *Quantum Chemistry* L, E — 5 CP	**30 CP**
2. Sem.	**MCh 20 1.1** *Advanced Inorganic Molecular and Solid State Chemistry* L, S — 10 CP	**MCh WP*** *Elective modules* 20 CP			**30 CP**
3. Sem.	**MCh WP*** *Elective modules* 20 CP	**MCh 20 3** *Focusing Laboratory Course* 10 CP			**30 CP**
4. Sem.	**MCh 20 4** *Master of Science Thesis* 30 CP				**30 CP**

* A total of 4 elective modules must be completed.

WP-modules in the winter term: WP 8, WP 9, WP 10, WP 11, WP 12, WP 13, WP 14, WP 15, WP 16 (duration: 2 semesters)

WP-modules in the summer term: WP 1, WP 2, WP 4, WP 5, WP 6, WP7, WP 17

Compulsory Modules

Advanced Inorganic Molecular and Solid State Chemistry Module No./ Code: MCh 20 1.1	UNIVERSITÄT BONN

1. Contents and Qualification Objectives	
Contents	• **Coordination chemistry**: mechanisms of reactions of coordination compounds (ligand exchange, electron transfer reactions) • **Reaction steps in homogeneous catalysis:** oxidative additions and reductive eliminations, σ-bond metatheses, insertion and elimination reactions • **Transition metal compounds**: metal hydrides and metal organyls, carbene complexes, olefin complexes (synthesis, structure, bonding and reactions) - metal activation of industrially relevant substrates, like dihydrogen, alkanes, carbon monoxide, olefins • **Main group element organyls**: element organyls of the boron group (triels) – hydroboration and carbometallation reactions • **Structural chemistry of inorganic solids**: structural arguments, packing types in solid compounds, phase transitions, systematic deduction of structures starting from dense sphere packings via filling of octahedral and tetrahedral gaps, molecular lattice, chain-structures, layered structures, network structures, diamandoid structures. • **Intermetallic phases and compounds**: alloys, Zintl phases and Zintl salts, polycationic and polyanionic clusters of the main group elements, Wade's rules • **Subvalent transition metal compounds**: magnetic phenomena, metal-metal bonding, metal-metal multiple bonding, metal clusters, condensation of clusters, metal rich compounds, cluster connection • **Solid-state materials**: precious stones, their use and production, diamond and diamond synthesis, fullerenes, carbon nanotubes, graphene • **Chemical bonding in solids**: introduction to the theory of electronic band structure, density of states, crystal orbitals.

Qualification Targets	• Acquisition of enhanced knowledge of the most important classes of modern inorganic molecular compounds
	• Develop a deeper understanding of
	  ○ transition metal hydrides, organyls and carbene complexes
	  ○ elementary steps in homogenous catalysis and in small molecule activation
	  ○ structure and structure-property relationships of solid state compounds
	• Advanced knowledge of concepts to describe the structure and chemical bonding in inorganic chemistry
	• Successful application of learning strategies
	• Use of the knowledge gained in the discussion of unknown compounds
	• Information management
	• Critical thinking
	• Problem-solving skills
	• Thorough knowledge and analytical skills for planning synthetic routes to complex chemical molecules
	• Analysis of and reflection on complex questions
	• Enhance ability to communicate

2. Course Format						
	Course Type	Topic	Language of Instruction	Group Size	Course Units	Workload [hr] (On-Site/ SLT)

					per Wee k	
	L	Advanced inorganic molecular and solid state chemistry	en.	60	6	180 (90 / 90)
	S	Seminar for the lecture	en.	20	2	120 (30 / 90)

3. Module Prerequisites	
Required	None
Recommended	

4. Module Application			
	Degree Program/ Component	Compulsory/ Elective	Program-Related Semester
	MSc Chemistry	Compulsory	1 or 2

5. Requirements for ECTS Credit Points		**6. ECTS CP**
Study Achievement(s)	None	**10**
Examinations and Examination Language	Written examination; en.	

7. Cycle		**8. Workload**	**9. Duration**
Winter semester ☒ Summer semester ☐	Winter and summer semester ☐	**300 hr**	**1 semester**

10. Module Organization	
Instructor	Prof. Dr. A.C. Filippou, Prof. Dr. J. Beck
Module Coordinator	Prof. Dr. A. C. Filippou
Organizational Unit Offering the Module	Department of Chemistry (FMNS), Institute for Inorganic Chemistry

11. Other	
Literature:	J. F. Hartwig, *Organotransition Metal Chemistry*, Univ. Science Books. R. H. Crabtree, *The Organometallic Chemistry Of The Transition Metals*, Wiley. C. Elschenbroich, *Organometallics*, Wiley-VCH. U. Müller, *Anorganische Strukturchemie*, Vieweg+Teubner Verlag. J. E. Huheey, E. A. Keiter, R. L. Keiter, *Anorganische Chemie: Prinzipien von Struktur und Reaktivität*, De Gruyter. L. H. Gade, *Koordinationschemie*, Wiley-VCH. F. A. Cotton, *Advanced Inorganic Chemistry*, Wiley. A. R. West, *Solid State Chemistry and its Applications*, Wiley

Organic Molecules and Materials Module No./ Code: MCh 20 1.2	

1. Contents and Qualification Objectives

Contents	• *Synthetic equivalent and "Umpolung:"* d/a nomenclature, Umpolung, acylanion equivalents • *Modern processes for C-C coupling reactions*: C-nucleophiles (enolates, metal organic reagents, transmetallation, homo- und cross coupling reactions), redox reactions • *Modern processes for C=C coupling*: Wittig and Wittig-like reactions, McMurry reaction, metal-induced olefin synthesis • *Stereoselective synthesis*: ex-chiral pool synthesis, chiral auxiliaries, enzymatic methods, enantioselective catalytical methods • *Retrosynthesis* • *Natural product synthesis*: protecting groups, total synthesis • Polymers (linear, branched, crosslinked, dendrimers) • Liquid crystals • Materials for electronic/optoelectronic applications (OTFTs, OLEDs, OPVs) • Modern analytical techniques • Primary and secondary metabolism • Enzyme classes and cofactors • Biosynthesis of fatty acids and polyketides • Biosynthesis of terpenes
Qualification Targets	• Detailed knowledge of key reactions and concepts in modern organic chemistry • Understanding of multistep reactions • Detailed knowledge of natural compound chemistry and material chemistry • Knowledge of modern analytical methods • Interpretation of chemical publications • Efficient learning strategies • Information management • Critical thinking • Problem solving skills • Thorough knowledge and analytical skills for planning synthetic routes to complex chemical molecules • Strengthen decision-making abilities • Strengthen reflectivity • Communication skills

2. Course Format

	Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr] (On-Site/ SLT)
	L	Synthetic chemistry, materials, natural products	en.	60	6	180 (90 / 90)
	S	Synthetic chemistry	en.	20	2	120 (30 / 90)

3. Module Prerequisites				
Required	None			
Recommended				
4. Module Application				
	Degree Program/ Component		Compulsory/ Elective	Program-Related Semester
	MSc Chemistry		Compulsory	1
5. Requirements for ECTS Credit Points				**6. ECTS CP**
Study Achievement(s)				**10**
Examinations and Examination Language	Written examination; en.			
7. Cycle		**8. Workload**	**9. Duration**	
Winter semester ☐ Summer semester ☐	Winter and summer semester ☒	**300 hr**	**1 semester**	
10. Module Organization				
Instructor	The instructors at the Kekulé Institute of Organic Chemistry and Biochemistry			
Module Coordinator	Prof. Dr. S. Höger			
Organizational Unit Offering the Module	Department of Chemistry (FMNS), Kekulé Institute of Organic Chemistry and Biochemistry			
11. Other				
Literature:	L. Kürti, B. Czakó, *Strategic Applications of Named Reactions in Organic Synthesis*, Elsevier. L. S. Hegedus, B. C. G. Söderberg, *Transition Metals in the Synthesis of Complex Organic Molecules*, University Science Books. F. A. Carey, R. J. Sundberg: *Advanced Organic Chemistry, Part A and B*, Springer. Further recommended literature will be announced in the courses.			

Advanced Physical Chemistry

Module No./ Code: MCh 20 1.3

UNIVERSITÄT BONN

1. Contents and Qualification Objectives

Contents	• **Structure formation**: models for nucleation, maturation, interfaces, membranes, aggregates, vesicles, protein/oligonucleotide folding and structure, and complex fluids • **Energetic excitations**: principle aspects, excitation coupling, energy transport and dissipation, application aspects • **Spectroscopy and imaging**: comparison of ensemble and single particle methods, space and time resolution, wave packet dynamics, optical methods, magnetic resonance, scanning probe techniques, Fourier transform in optics and spectroscopy
Qualification Targets	• Application of thermodynamical principles and spectroscopic methods from bachelor's program to complex systems • Consolidation and extension of model formation skills and development of concepts for the description of complex matter • Acquisition of knowledge of advanced spectroscopic and microscopic analysis techniques • Assessment of methods for solving physico-chemical problems • Analytical problem solving competence • Critical thinking

2. Course Format

	Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr] (On-Site/ SLT)
	L	Advanced topics in physical chemistry	en.	60	2	75 (30 / 45)
	E	Exercise for the lecture	en.	20	2	75 (30 / 45)

3. Module Prerequisites

Required	None
Recommended	

4. Module Application

	Degree Program/ Component	Compulsory/ Elective	Program-Related Semester
	MSc Chemistry	Compulsory	1

5. Requirements for ECTS Credit Points | 6. ECTS CP

		6. ECTS CP
Study Achievement(s)	50% of the achievable credits are for the exercises	5
Examinations and Examination Language	Written examination; en.	

7. Cycle | 8. Workload | 9. Duration

7. Cycle		8. Workload	9. Duration
Winter semester ☐ Summer semester ☐	Winter and summer semester ☒	**150 hr**	**1 semester**

10. Module Organization	
Instructor	The instructors at the Institute of Physical and Theoretical Chemistry
Module Coordinator	Prof. Dr. U. Kubitscheck
Organizational Unit Offering the Module	Department of Chemistry (FMNS), Institute of Physical and Theoretical Chemistry
11. Other	
Literature:	C. Rullière, *Femtosecond Laser Pulses*, Springer. H. Kuhn, H.-D. Försterling, D. H. Waldeck, *Principles Of Physical Chemistry*, Wiley. W. Demtröder, *Laserspektroskopie*, Springer. K. Dill, S. Bromberg, *Molecular Driving Forces: Statistical Thermodynamics in Biology, Chemistry, Physics, and Nanoscience*, Garland Science. E. Kreyszig, *Advanced Engineering Mathematics*, Wiley

Quantum Chemistry

Module No./ Code: MCh 20 1.4

UNIVERSITÄT BONN

1. Contents and Qualification Objectives

Contents	This module provides an introduction to modern calculation methods for quantum chemistry. It provides methodical knowledge that chemists absolutely need today to understand the literature and provide theoretical support for their own studies. The module is based on a new concept that aims to present quantum chemistry from a qualitative chemistry point of view, but without neglecting the mathematical steps required for a quantitative description of molecules and their properties. Therefore, the mathematical formulas as well as chemical concepts and their relation to quantum chemical quantities are discussed in detail. In particular, the distinction between measurable properties (observables) and qualitative concepts is emphasized. Furthermore, the route from a physical model to its mathematical formulation, algorithmic implementation and subsequent application will be a central point. **Contents** • Introduction to the quantitative description of electronic structure • Hartree-Fock and basis sets • Total energies, electron densities, orbital energies and orbitals • Qualitative electronic structure of molecules in the MO model; population analyses • Hückel models and semi-empirical MO methods • Basics of wave function based electron correlation methods • Geometry optimization and potential energy surfaces • Basics and applications of density functional theory • Thermochemistry
Qualification Targets	• Basic knowledge of the qualitative and quantitative description of the electronic structure of molecules and their chemical and physical properties • Understanding of modern calculation methods in theoretical chemistry • Application and critical assessment of the theoretical models learned and methods for the computational or phenomenological solution of chemical problems • Learning competence • Methodological competence • Self-competence

2. Course Format

	Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr] (On-Site/ SLT)
	L	Quantum chemistry	en.	60	2	75 (30 / 45)
	E	Exercise for the lecture	en.	20	2	75 (30 / 45)

3. Module Prerequisites

Required	None
Recommended	

<table>
<tr><th colspan="5">4. Module Application</th></tr>
<tr><td rowspan="2"></td><td colspan="2">Degree Program/ Component</td><td>Compulsory/ Elective</td><td>Program-Related Semester</td></tr>
<tr><td colspan="2">MSc Chemistry</td><td>Compulsory</td><td>1</td></tr>
<tr><th colspan="4">5. Requirements for ECTS Credit Points</th><th>6. ECTS CP</th></tr>
<tr><td>Study Achievement(s)</td><td colspan="3">50% of the achievable credits are for the exercises</td><td rowspan="2">5</td></tr>
<tr><td>Examinations and Examination Language</td><td colspan="3">Written examination; en.</td></tr>
<tr><th colspan="2">7. Cycle</th><th>8. Workload</th><th colspan="2">9. Duration</th></tr>
<tr><td>Winter semester ☐
Summer semester ☐</td><td>Winter and summer semester ☒</td><td>150 hr</td><td colspan="2">1 semester</td></tr>
<tr><th colspan="5">10. Module Organization</th></tr>
<tr><td>Instructor</td><td colspan="4">Prof. Dr. S. Grimme, Dr. A. Hansen</td></tr>
<tr><td>Module Coordinator</td><td colspan="4">Prof. Dr. S. Grimme</td></tr>
<tr><td>Organizational Unit Offering the Module</td><td colspan="4">Department of Chemistry (FMNS), Institute of Physical and Theoretical Chemistry</td></tr>
<tr><th colspan="5">11. Other</th></tr>
<tr><td>Literature:</td><td colspan="4">F. Jensen, Introduction to Computational Chemistry, Wiley.</td></tr>
</table>

Analytical Methods for Condensed Matter

Module No./ Code: MCh 20 2

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1. Contents and Qualification Objectives

Contents	• Basic concepts of crystallography • Physical principles of the phenomena of diffraction of X-rays and electrons • Application of these methods to determine the structure of crystalline and non-crystalline materials • Vibrational spectroscopy for solid compounds, factor group analysis • Electronic spectra and magnetism of transition metal compounds
Qualification Targets	• Ability to apply the knowledge achieved to the interpretation of diffraction patterns and structure determination • Development of problem-solving abilities and expansion of analytical skills • Acquisition of methodical and apparatus knowledge • Critical assessment of results • Recognizing the limitations of scientific methods • Recognizing pitfalls and avoiding unsuitable interpretations • Training of the spatial sense

2. Course Format

Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr] (On-Site/ SLT)
L	Advanced analytical methods in inorganic chemistry	en.	60	3	120 (45 / 75)
S	Seminar for the lecture	en.	60	2	90 (30 / 60)
LC	Practical exercises for the lecture topics	en.	2	3	90 (45 / 45)

3. Module Prerequisites

Required	None
Recommended	

4. Module Application

Degree Program/ Component	Compulsory/ Elective	Program-Related Semester
MSc Chemistry	Compulsory	1 or 2

5. Requirements for ECTS Credit Points

		6. ECTS CP
Study Achievement(s)	50% of the achievable credits are for the exercises	10
Examinations and Examination Language	Written examination; en.	

7. Cycle		8. Workload	9. Duration
Winter semester ☐ Summer semester ☒	Winter and summer semester ☐	**300 hr**	**1 semester**

10. Module Organization	
Instructor	The instructors at the Institute for Inorganic Chemistry
Module Coordinator	Prof. Dr. J. Beck
Organizational Unit Offering the Module	Department of Chemistry (FMNS), Institute for Inorganic Chemistry
11. Other	
Literature:	W. Massa *Kristallstrukturbestimmung*, Springer-Verlag. W. Massa*, Crystal Structure determination*, Springer. C. Hammond, *The Basics of Crystallography and Diffraction*, IUCr Publishers. W. Borchardt-Ott, H. Sowa, *Kristallographie*, Springer. K. Nakamoto, *Infrared and Raman Spectra*, Wiley. C. E. Housecroft, A. G. Sharpe, Inorganic Chemistry, Pearson.

Focusing Laboratory Course

Module No./ Code: MCh 20 3

UNIVERSITÄT BONN

1. Contents and Qualification Objectives

Contents	In this module, students are supposed to learn how to work independently on a scientific topic in an experimental or theoretical manner by conducting a self-contained scientific project study. For this purpose, the student shall join an active scientific working group. The module's accompanying seminar imparts the basic and advanced knowledge needed for the particular topic. Extensive literature research which includes the main topic as well as related and adjacent issues shall be the basis for this. Students summarize the results of the experimental work as well as those of the literature research in a written report. They also present their results in an oral presentation. This module can prepare for a master's thesis.
Qualification Targets	• Preparation for theoretical and practical scientific work during the master's thesis • Independent scientific work • Independent use of the possibilities of (literature) research in order to acquire full state of knowledge of a topic • Ability to present own scientific work to a professional as well as a lay audience • Efficient time management • Information management • Organizational skills • Further development of communication skills

2. Course Format

	Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr][1]
	LC		en.	1		270
	S		en.	1		30

3. Module Prerequisites

Required	Passed modules MCh 20 1.2, MCh 20 1.3, MCh 20 1.4 and one passed elective module from WP 1 to WP 17
Recommended	

4. Module Application

	Degree Program/ Component	Compulsory/ Elective	Program-Related Semester
	MSc Chemistry	Compulsory	2 or 3

5. Requirements for ECTS Credit Points / 6. ECTS CP

		6. ECTS CP
Study Achievement(s)	None	10
Examinations and Examination Language	Presentation (40%) and report (60%); en.	

7. Cycle		8. Workload	9. Duration
Winter semester ☐ Summer semester ☐	Winter and summer semester ☒	**300 hr**	**1 semester**

10. Module Organization

Instructor	The instructors at the Department of Chemistry (FMNS) and others
Module Coordinator	The supervisor chosen by the student

Organizational Unit Offering the Module	Department of Chemistry (FMNS) and others
11. Other	
Notes:	[1]: Distribution of the workload between on-site and self-study time is different for each student and is determined in consultation with the student's supervisor.

Master's Thesis

Module No./ Code: MCh 20 4

1. Contents and Qualification Objectives						
Contents	The topics of the master's thesis are assigned by the supervisor chosen by the student.					
Qualification Targets	By writing the master's thesis, students should demonstrate that they are able to develop and present scientific findings in writing within a time frame of six months using the knowledge and methods of modern chemical research acquired during their previous studies. Own results should be included, discussed and evaluated in an appropriate way. The following key competences should be addressed: • Ability to work independently on a scientific topic • Writing skills • Self-management, self-organization, self-motivation • Critical thinking • Ability to collect, understand, analyze and mentally connect information • Efficient time management					
2. Course Format						
	Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr]
	Independent work		en.	1		900[1]
3. Module Prerequisites						
Required	Passed modules MCh 20 1.1, MCh 20 1.2, MCh 20 1.3, MCh 20 1.4, MCh 20 2 and a total of 60 CP from the module examinations for the master's program in Chemistry					
Recommended						
4. Module Application						
	Degree Program/ Component	Compulsory/ Elective	Program-Related Semester			
	MSc Chemistry	Compulsory	3 or 4			
5. Requirements for ECTS Credit Points		**6. ECTS CP**				
Study Achievement(s)	Oral presentation of the results of the master's thesis	**30**				
Examinations and Examination Language	Master's thesis; en.					
7. Cycle		**8. Workload**	**9. Duration**			
Winter semester ☐ Summer semester ☐	Winter and summer semester ☒	**900 hr**	**1 semester**			
10. Module Organization						
Instructor	The instructors at the Faculty of Chemistry (FMNS)					
Module Coordinator	The supervisor chosen by the student					
Organizational Unit Offering the Module	Department of Chemistry (FMNS)					
11. Other						
Notes:	[1]: Distribution of the workload between on-site and self-study time is different for each student and is determined in consultation with the student's supervisor.					

Elective Modules

Industrial Inorganic Molecular Chemistry Module No./ Code: MCh 20 WP 1	UNIVERSITÄT BONN
1. Contents and Qualification Objectives	
Contents	**Lecture Part Transition Metal Chemistry (60 hr):** • Catalytic hydroformylation • Catalytic hydrogenation • Catalytic olefin polymerization • Catalytic hydrocyanation, hydrosilylation and hydroamination • Alkene and alkyne metathesis **Lecture Part Main Group Chemistry (60 hr):** • Introduction to heteronuclear NMR spectroscopy (II) (^{7}Li, ^{11}B, ^{19}F, ^{29}Si and ^{31}P; hetero- and homonuclear E,E' couplings; structure discussion) • Boron compounds: boranes, hydroboration, trihaloboranes, iminoboranes, borazine, boron clusters, carboboranes • Aluminum compounds: synthesis and reaction of MAO (mechanism of Ziegler-Natta polymerization) • Gallium and Indium compounds as single-source precursors for MOCVD • Silicon compounds: diorganodichlorosilanes (Wacker process); silylenes, disilenes, polysilanes; silanols, and polysiloxanes • Tin compounds: triorganylstannanes (hydrostannylation) • Phosphorus compounds: synthesis of P^{III} ligands (complexes, use in catalyses), aminophosphanes, phosphazenes, polyphosphazenes; Wittig ylides (organic C1 building blocks); phosphaalkenes and -alkynes as new P-C building blocks **Lab course (optional):** • Syntheses and reactivity studies of molecular transition metal and main group element compounds under inert gas conditions (Schlenk, vacuum line and glove box techniques) • Training in purification and characterization methods under strictly anaerobic conditions • Purification methods: vacuum distillation, vacuum sublimation, crystallization, column chromatography under strictly anaerobic conditions • Characterization methods: heteronuclear NMR-, IR-, Raman-, and UV-Vis spectroscopy, mass spectrometry, cyclic voltammetry, single-crystal X-ray diffraction • SciFinder/Beilstein searches • Houben/Weyl (Science of Synthesis) • Chemical Abstracts

<table>
<tr><td>Qualification Targets</td><td colspan="6">Acquisition of advanced knowledge in the field of molecular inorganic chemistry and homogeneous catalysis
In-depth understanding of the bonding, structure, reactions and industrial use of transition metal and main group element compounds
Consolidation of knowledge of spectroscopic methods and their application in molecular inorganic chemistry
In-depth knowledge of molecular transition metal and main group element compounds and their application in industrial processes
Advanced knowledge of analytical and spectroscopic techniques, and their application in molecular inorganic chemistry
Training in special experimental techniques for the preparation and characterization of highly air- and moisture-sensitive compounds</td></tr>
<tr><td colspan="7">2. Course Format</td></tr>
<tr><td rowspan="3"></td><td>Course Type</td><td>Topic</td><td>Language of Instruction</td><td>Group Size</td><td>Course Units per Week</td><td>Workload [hr] (On-Site/ SLT)</td></tr>
<tr><td>L</td><td>Industrial inorganic molecular chemistry</td><td>en.</td><td>30</td><td>4</td><td>150 (60 / 90)</td></tr>
<tr><td>S</td><td>Seminar for the lecture</td><td>en.</td><td>20</td><td>4</td><td>150 (60 / 90)</td></tr>
<tr><td colspan="7">3. Module Prerequisites</td></tr>
<tr><td>Required</td><td colspan="6">Passed module MCh 20 1.1</td></tr>
<tr><td>Recommended</td><td colspan="6"></td></tr>
<tr><td colspan="7">4. Module Application</td></tr>
<tr><td rowspan="2"></td><td colspan="4">Degree Program/ Component</td><td>Compulsory/ Elective</td><td>Program-Related Semester</td></tr>
<tr><td colspan="4">MSc Chemistry</td><td>Elective</td><td>2 or 3</td></tr>
<tr><td colspan="6">5. Requirements for ECTS Credit Points</td><td>6. ECTS CP</td></tr>
<tr><td>Study Achievement(s)</td><td colspan="5">Exercises and seminar presentation</td><td rowspan="2">10</td></tr>
<tr><td>Examinations and Examination Language</td><td colspan="5">Final oral examination; en.</td></tr>
<tr><td colspan="2">7. Cycle</td><td colspan="2">8. Workload</td><td colspan="3">9. Duration</td></tr>
<tr><td>Winter semester ☐
Summer semester ☒</td><td colspan="2">Winter and summer semester ☐</td><td colspan="2">300 hr</td><td colspan="2">1 semester</td></tr>
<tr><td colspan="7">10. Module Organization</td></tr>
<tr><td>Instructor</td><td colspan="6">Prof. Dr. A. C. Filippou, Prof. Dr. R. Streubel</td></tr>
<tr><td>Module Coordinator</td><td colspan="6">Prof. Dr. A. C. Filippou</td></tr>
<tr><td>Organizational Unit Offering the Module</td><td colspan="6">Department of Chemistry (FMNS), Institute for Inorganic Chemistry</td></tr>
<tr><td colspan="7">11. Other</td></tr>
<tr><td>Literature:</td><td colspan="6">J. F.Hartwig, Organotransition Metal Chemistry, Univ. Science Books.
D. Steinborn, Grundlagen der metallorganischen Komplexkatalyse, Vieweg+Teubner Verlag.</td></tr>
</table>

Supramolecular Chemistry Module No./ Code: MCh 20 WP 2	UNIVERSITÄT BONN

1. Contents and Qualification Objectives	
Contents	• Historical development of the field of supramolecular chemistry • Terms and definitions • Non-covalent interactions • Characterization of supramolecular binding phenomena • Binding constants and other thermodynamic data • Analytical tools • Recognition of ionic substrates – cations, anions, and ion pairs • Recognition of neutral substrates – privileged structural motifs and binding motifs • Recognition of chiral substrates • Self-assembly processes – basic considerations • Self-assembly via hydrogen bonding • Coordination-driven self-assembly • Surface patterning • Supramolecular control of reactivity • Rotaxanes, catenanes, knots, and molecular machines • Dendrimers • Applications as sensors
Qualification Targets	• Basic knowledge of the concepts of supramolecular chemistry in theory and practice • Knowledge of the different types of non-covalent interactions and their deliberate application in molecular recognition and supramolecular aggregation • Advanced laboratory practices • Advanced knowledge of modern analytical techniques • Written documentation of scientific results • Efficient time management • Information management • Organizational skills • Further training of experimental skills • Further training of observation skills • Development of problem solving skills • Development of analytical skills, e.g. interpretations of experimental findings concerning supramolecular phenomena • Further development of decision making skills • Further training of accuracy and responsibility • Further development of communication skills • Further training of (self-) critical assessment

2. Course Format						
	Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr]
	L/S	Supramolecular chemistry	en.	30	4	120 (60 / 60)
	LC	Experiments on lecture/seminar topics	en.	2	6	180 (90 / 90)

3. Module Prerequisites			
Required	Passed module MCh 20 1.2		
Recommended			
4. Module Application			
	Degree Program/ Component	Compulsory/ Elective	Program-Related Semester
	MSc Chemistry	Elective	2 or 3
5. Requirements for ECTS Credit Points			**6. ECTS CP**
Study Achievement(s)	Successful completion of lab course		**10**
Examinations and Examination Language	Final oral examination; en.		

7. Cycle		**8. Workload**	**9. Duration**
Winter semester ☐ Summer semester ☒	Winter and summer semester ☐	**300 hr**	**1 semester**

10. Module Organization	
Instructor	Prof. Dr. A. Lützen, Dr. S.-S. Jester, Dr. L. von Krbek
Module Coordinator	Prof. Dr. A. Lützen
Organizational Unit Offering the Module	Department of Chemistry (FMNS), Kekulé Institute of Organic Chemistry and Biochemistry
11. Other	
Literature:	J. W. Steed, J. L. Atwood, *Supramolecular Chemistry*, John Wiley & Sons. Further recommended literature will be announced in the courses.

Advanced Quantum Chemistry Methods Module No./ Code: MCh 20 WP 4	UNIVERSITÄT BONN

1. Contents and Qualification Objectives	
Contents	The module addresses students with strong interest in the theoretical treatment of molecules, molecular properties and chemical reactions. After the recapitulation of HF-theory and the introduction of fundamental new concepts for the treatment of the N-electron problem, the standard methods of correlated ab initio quantum chemistry (CI, MP, CC) are discussed. The numerical accuracy of the various methods will be documented using benchmark results for small molecules. Necessary steps for implementation of the methods are shown using examples and the algorithmic efficiency of different software implementations and special treatments for large systems are demonstrated. Other key topics are density functional theory and approximate functionals, their properties and limits as well as non-covalent interactions. Introduction to further topics, e.g. quantum dynamics, treatment of heavy elements, and electronically excited states. The associated practical programming course provides the opportunity for preparing a simple HF- and MP2 program yielding insight into the practical aspects and deepening the theoretical knowledge from the lecture. In its second part, various typical chemical problems (structure, thermochemistry, spectroscopy) will be treated with standard quantum chemistry codes. **Contents:** • Recapitulation of Hartree-Fock theory • Efficient methods for large systems • Qualitative discussion of the electron correlation problem • Second quantization and diagrammatic techniques • Wave function based correlation methods (CI, MP, CC) • Basis set extrapolation and explicit correlation • Relativistic effects and effective potentials • Density functional theory • Theoretical spectroscopy and molecular properties • Electronically excited states, multi-reference methods • Quantum dynamics • Non-covalent interactions and dispersion corrections
Qualification Targets	• Detailed knowledge of methods and concepts in quantum chemistry for the quantitative treatment of the electronic structure of atoms and molecules • Introduction into the programming language Fortran and implementation of quantum chemical methods in computer programs • Practical calculations and interpretation of quantum chemical treatments • Preparation for independent work in the area of quantum chemistry • Learning competence • Methodological competence • Self-competence

2. Course Format						
	Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr] (On-Site/ SLT)
	L	Quantum chemistry II	en.	20	2	60 (30 / 30)
	S	Seminar for the lecture	en.	20	2	80 (30 / 50)
	LC	Experiments on lecture/seminar topics	en.	1	5	160 (75 / 85)

3. Module Prerequisites	
Required	Passed module MCh 20 1.4
Recommended	

4. Module Application			
	Degree Program/ Component	Compulsory/ Elective	Program-Related Semester
	MSc Chemistry	Elective	2 or 3

5. Requirements for ECTS Credit Points		**6. ECTS CP**
Study Achievement(s)	Successful completion of the lab course and seminar presentation	**10**
Examinations and Examination Language	Final oral examination; en.	

7. Cycle		**8. Workload**	**9. Duration**
Winter semester ☐ Summer semester ☒	Winter and summer semester ☐	**300 hr**	**1 semester**

10. Module Organization	
Instructor	Prof. Dr. S. Grimme, Dr. A. Hansen
Module Coordinator	Prof. Dr. S. Grimme
Organizational Unit Offering the Module	Department of Chemistry (FMNS), Institute of Physical and Theoretical Chemistry

11. Other	
Literature:	A. Szabo, N. S. Ostlund, *Modern Quantum Chemistry*. T Helgaker, P. Jørgensen, J. Olsen, *Molecular Electronic Structure Theory*, Wiley.

Surface Science and Electrochemistry

Module No./ Code: MCh 20 WP 5

UNIVERSITÄT BONN

1. Contents and Qualification Objectives

Contents	• Thermodynamics of interfaces and surfaces • Geometric and electronic structures of interfaces • Adsorption and desorption processes • Chemical binding to surfaces • Mechanism of heterogeneous catalysis • Experimental methods for surface analysis • Layer growth and nucleation • Models of the electric double layer • Electrochemical kinetics, Marcus theory • Electrocatalysis • Electrochemical methods • Electrochemical in situ characterization • Technical applications of processes at interfaces
Qualification Targets	• Properties, concepts, and models in surface chemistry and electrochemistry. • Experimental methods for the investigation of surfaces and electrochemical interfaces and related chemical processes. • Understanding and applying concepts and models • Conducting experimental investigations • Basic understanding of modern research literature

2. Course Format

	Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr] (On-Site/ SLT)
	L	Surface science and electrochemistry	en.	30	3	135 (45 / 90)
	S	Seminar for the lecture	en.	30	1	45 (15 / 30)
	LC	Experiments on lecture/seminar topics	en.	2	4	120 (60 / 60)

3. Module Prerequisites

Required	Passed module MCh 20 1.3
Recommended	

4. Module Application

	Degree Program/ Component	Compulsory/ Elective	Program-Related Semester
	MSc Chemistry	Elective	2 or 3

5. Requirements for ECTS Credit Points — 6. ECTS CP

		6. ECTS CP
Study Achievement(s)	Certificates of attendance for the lab course and lab reports	10
Examinations and Examination Language	Written examination; en.	

7. Cycle		8. Workload	9. Duration
Winter semester ☐ Summer semester ☒	Winter and summer semester ☐	**300 hr**	**1 semester**

10. Module Organization	
Instructor	Prof. Dr. M. Sokolowski
Module Coordinator	Prof. Dr. M. Sokolowski
Organizational Unit Offering the Module	Department of Chemistry (FMNS), Institute of Physical and Theoretical Chemistry

11. Other	
Literature:	G. Attard, C. Barnes, *Surfaces*, Oxford Univ. Press. K. W. Kolasinski, *Surface Science: Foundations of Catalysis and Nonoscience*, Wiley. W. Schmickler, E. Santos, *Interfacial Electrochemistry*, Springer. D. Pletcher, Southampton Electrochemistry Group, *Instrumental Methods in Electrochemistry*, Elsevier Science & Technology. C. H. Hamann, A. Hamnett, W. Vielstich, *Electrochemistry*, Wiley-VCH.

Chemical Biology / Medicinal Chemistry Module No./ Code: MCh 20 WP 6	UNIVERSITÄT BONN

1. Contents and Qualification Objectives	
Contents	**Theory:** • Synthesis and exploitation of drugs • Interaction of drugs with target proteins, functional in vitro assays • Synthesis, structure and applications of nucleic acids, peptides and proteins • Organic chemistry of enzyme-catalyzed reactions • Glycochemistry • Lipids and chemistry of membranes • Strategies for drug research • Catalytic antibodies • Combinatorial chemistry and biochemistry • Phage and ribosome display • Aptamers • Ribosomal RNA technologies • Models concerning the origin of life **Lab course:** • Interaction analysis of drugs with target proteins • Taq polymerase/PCR primer design • Kinetics of enzyme-catalyzed reactions • HPLC/MS • Gel shift assays • Fluorescence Resonance Energy Transfer • Functional enzyme assays • Synthesis of a drug • Isolation of a pharmacologically active natural product
Qualification Targets	• Knowledge of the synthesis and properties of biopolymers • Knowledge of current methods in bioorganic chemistry, combinatorial chemistry, medicinal chemistry and chemical biology • Application of the concepts to modern biological and biotechnological problems

2. Course Format

	Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr] (On-Site/ SLT)
	L	Medical chemistry and chemical biology	en.	6	3	90 (45 / 45)
	S	Seminar for the lecture	en.	6	0.5	20 (7.5 / 12.5)
	LC	Experiments on lecture/seminar topics	en.	2	5.5	190 (82.5 / 107.5)

3. Module Prerequisites	
Required	Passed module MCh 20 1.2
Recommended	

4. Module Application			
	Degree Program/ Component	Compulsory/ Elective	Program-Related Semester
	MSc Chemistry	Elective	2 or 3
	B. Sc. Molecular Biomedicine	Elective	

5. Requirements for ECTS Credit Points		**6. ECTS CP**
Study Achievement(s)	Lab reports	**10**
Examinations and Examination Language	Written examination; en.	

7. Cycle		**8. Workload**	**9. Duration**
Winter semester ☐ Summer semester ☒	Winter and summer semester ☐	**300 hr**	**1 semester**

10. Module Organization	
Instructor	Prof. Dr. C. E. Müller, Prof. Dr. M. Gütschow, Prof. Dr. M. Famulok, Prof. Dr. G. Mayer
Module Coordinator	Prof. Dr. C. E. Müller
Organizational Unit Offering the Module	Department of Molecular Biomedicine (FMNS); Department of Pharmacy (FMNS)

11. Other	
Literature:	A. Miller, J. Tanner, *Essentials of Chemical Biology: Structure and Dynamics of Biological Macromolecules*, Wiley. G. L. Patrick, *An Introduction to Medicinal Chemistry*, Oxford University Press.

Organometallic Chemistry Module No./ Code: MCh 20 WP 7	UNIVERSITÄT BONN

1. Contents and Qualification Objectives

Contents	**Theory:** • Fundamentals of catalysis • Application of modern catalytic methods for the synthesis of complex organic compounds • Discussion of reaction mechanisms with respect to selectivity • Discussion of essential aspects of sustainability for the large-scale and industrial-scale application of catalytic reactions. Feed stock substrates. • Discussion of diversity oriented synthesis in the context of catalyst controlled reactions **Lab course:** • Selected aspects of laboratory practice: Reaction control, automated chromatography, HPLC, reaction optimization • Product identification by NMR, determination of enantiomeric ratios by HPLC • Interactive discussion of reaction mechanisms
Qualification Targets	• Detailed knowledge of modern organometallic reactions • Understanding and evaluation of complex organometallic mechanisms and their influence on selectivity • Key concepts of catalysis with open-shell intermediates • Advanced laboratory practices • Written documentation of scientific results • Efficient time management • Information management • Organizational skills • Further training of experimental skills • Further training of observation skills • Development of problem solving skills • Development of analytical skills, e.g. application of concepts of organometallic chemistry and independent understanding of complex reactions for advanced applications in organic synthesis • Further development of decision making skills • Further training of accuracy and responsibility • Further development of communication skills • Further training of (self-) critical assessment

2. Course Format

	Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr] (On-Site/ SLT)
	L	Organometallic chemistry	en.	30	4	150 (60 / 90)
	LC	Experiments on lecture topics	en.	1–5	6	150 (90 / 60)

3. Module Prerequisites

Required	Passed module MCh 20 1.2
Recommended	

<table>
<tr><td colspan="5">4. Module Application</td></tr>
<tr><td rowspan="2"></td><td colspan="2">Degree Program/ Component</td><td>Compulsory/ Elective</td><td>Program-Related Semester</td></tr>
<tr><td colspan="2">MSc Chemistry</td><td>Elective</td><td>2 or 3</td></tr>
<tr><td colspan="4">5. Requirements for ECTS Credit Points</td><td>6. ECTS CP</td></tr>
<tr><td>Study Achievement(s)</td><td colspan="3">Lab report</td><td rowspan="2">10</td></tr>
<tr><td>Examinations and Examination Language</td><td colspan="3">Written examination; en.</td></tr>
<tr><td colspan="2">7. Cycle</td><td>8. Workload</td><td colspan="2">9. Duration</td></tr>
<tr><td>Winter semester ☐
Summer semester ☒</td><td>Winter and summer semester ☐</td><td>300 hr</td><td colspan="2">1 semester</td></tr>
<tr><td colspan="5">10. Module Organization</td></tr>
<tr><td>Instructor</td><td colspan="4">Prof. Dr. A. Gansäuer</td></tr>
<tr><td>Module Coordinator</td><td colspan="4">Prof. Dr. A. Gansäuer</td></tr>
<tr><td>Organizational Unit Offering the Module</td><td colspan="4">Department of Chemistry (FMNS), Kekulé Institute of Organic Chemistry and Biochemistry</td></tr>
<tr><td colspan="5">11. Other</td></tr>
<tr><td>Literature:</td><td colspan="4">L. S. Hegedus, B. C. G. Söderberg, Transition Metals in the Synthesis of Complex Organic Molecules, University Science Books.

Further recommended literature will be announced in the courses.</td></tr>
</table>

Molecular Dynamics of Time Dependent Phenomena Module No./ Code: MCh 20 WP 8	UNIVERSITÄT BONN

1. Contents and Qualification Objectives

Contents	• **Monoatomic Systems:** Newtonian dynamics, integrational algorithms, properties; thermodynamical state control: constant temperature, constant pressure; free energy calculations (thermodynamical integration); molecular systems: intramolecular forces, long range forces; advanced methods: polarizable force fields, molecular dynamics simulations, entropy, reactions, state of the art methods and tools are used to calculate correlation functions, vibrational spectra for the structure of systems in most cases of condensed matter (e.g. liquids and solvent effects). • **Quantum Dynamics:** numerical propagation of the time-dependent Schrödinger equation in the absence/presence of electric fields, semi-classical approach to linear and non-nonlinear optical spectroscopy, time-dependent Franck-Condon factor, transient absorption and stimulated emission, bound-to-bound and bound-to-free transitions, Femto-chemistry and photodissociation of triatomic molecules/ions. • **Ultrafast Laser Spectroscopy**: properties of ultrafast optical pulses, phase velocity versus group velocity, phase delay versus group delay, phase velocity dispersion versus group velocity dispersion, higher-order dispersions, spectral amplitude and spectral phase, electric field autocorrelation function, interferometric and background-free intensity autocorrelation function, frequency-resolved optical gating, pump-probe spectroscopy. • **Ultrafast Laser Laboratory:** conducting experiments using a Kerr-lens mode-locked femtosecond Ti:Sapphire laser pumped by a frequency-doubled Nd:YVO4 laser. Measuring the group delay of optically transmissive materials using a correlation pump-probe experiment. Learning the operating principles of lasers, photon detectors, lock-in amplifiers and opto-mechanical components.
Qualification Targets	• Advanced knowledge of modern theoretical and experimental methods of time dependent spectroscopy, wave packet dynamics and molecular dynamics • Understanding of the interaction between theory and experiment • Independent performance and analysis of ultrafast laser experiments • Application of knowledge to solve critically theoretical and practical problems, e.g. programming and oral presentations

2. Course Format

	Course Type	Topic	Language of Instruction	Group Size	Cours e Units per Week	Workload [hr] (On-Site/ SLT)
	L	Molecular dynamics simulations, quantum dynamics	en.	30	2	60 (30 / 30)
	S	Seminar on lecture topics	en.	30	2	80 (30 / 50)
	LC	Experiments on lecture topics	en.	3	4	160 (60 / 100)

3. Module Prerequisites			
Required	Passed module MCh 20 1.3		
Recommended			
4. Module Application			
	Degree Program/ Component	Compulsory/ Elective	Program-Related Semester
	MSc Chemistry	Elective	2 or 3

5. Requirements for ECTS Credit Points		**6. ECTS CP**
Study Achievement(s)	Lab report	**10**
Examinations and Examination Language	Final oral examination; en.	

7. Cycle		**8. Workload**	**9. Duration**
Winter semester ☒ Summer semester ☐	Winter and summer semester ☐	**300 hr**	**1 semester**

10. Module Organization	
Instructor	Prof. Dr. B. Kirchner, Prof. Dr. P. Vöhringer
Module Coordinator	Prof. Dr. B. Kirchner, Prof. Dr. P. Vöhringer
Organizational Unit Offering the Module	Department of Chemistry (FMNS), Institute of Physical and Theoretical Chemistry
11. Other	
Literature:	D. Frenkel, B. Smit, *Understanding Molecular Simulation*, Acad. Press. M. P. Allen, D. J. Tildesley, *Computer Simulation of Liquids*, Clarendon Press. G. Fleming, *Chemical Applications of Ultrafast Spectroscopy*, U. S. Oxford Univ. Press. S. Mukamel, *Principles of Nonlinear Optical Spectroscopy*, Oxford Univ. Press.

Macromolecular Chemistry Module No./ Code: MCh 20 WP 9	UNIVERSITÄT BONN
1. Contents and Qualification Objectives	

Contents	**Theory:** • Polymerizations, molecular weight and its determination • Chain conformation, rubber elasticity • Phase transitions in polymers (Tm, Tg), viscoelasticity • Step growth polymerizations (polyesters, polyamides, polysiloxanes, polyurethanes, dendrimers, conjugated polymers) • Polycondensation kinetics • Controlled reactions • Radical polymerization, homopolymers (kinetics, molecular weight), chain transfer, copolymers, emulsion polymerization, controlled radical polymerization • Anionic polymerization, polyacrylates • Characterization (viscosity, GPC, osmometry, light scattering, MALDI- TOF spectrometry, NMR) • Cationic polymerization • Polyolefins • Metathesis polymerization (ROMP, ADMET) • Crystallinity in polymers • Supramolecular polymers • Processing and recycling • Industrial aspects of polymer chemistry **Lab course:** Selection of experiments on the following topics: • Radical bulk polymerization • Molecular weight and transfer agents • Emulsion polymerization • Controlled radical polymerization • Polycondensation, polyaddition • Viscosity • Gel permeation chromatography (GPC) • Phase transitions in polymers (DTA, DSC) • Rubber elasticity

Qualification Targets	• Knowledge of synthesis, properties and applications of polymers • Knowledge of modern methods to characterize polymers • Advanced laboratory practices • Written documentation of scientific results • Efficient time management • Information management • Organizational skills • Further training of experimental skills • Further training of observation skills • Development of problem solving skills • Development of analytical skills, e.g. application of concepts of macromolecular chemistry for an independent synthesis and characterization of polymers • Further development of decision making skills • Further training of accuracy and responsibility • Further development of communication skills • Further training of (self-) critical assessment

2. Course Format

Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr] (On-Site/ SLT)
L/S	Macromolecular chemistry	en.	30	4	150 (60 / 90)
LC	Experiments on lecture topics	en.	2–3	4	150 (60 / 90)

3. Module Prerequisites

Required	Passed module MCh 20 1.2
Recommended	

4. Module Application

Degree Program/ Component	Compulsory/ Elective	Program-Related Semester
MSc Chemistry	Elective	2 or 3

5. Requirements for ECTS Credit Points		**6. ECTS CP**
Study Achievement(s)	Lab reports	**10**
Examinations and Examination Language	Written examination; en.	

7. Cycle		**8. Workload**	**9. Duration**
Winter semester ☒ Summer semester ☐	Winter and summer semester ☐	**300 hr**	**1 semester**

10. Module Organization

Instructor	Prof. Dr. S. Höger, Dr. Gabriele Richardt
Module Coordinator	Prof. Dr. S. Höger
Organizational Unit Offering the Module	Department of Chemistry (FMNS), Kekulé Institute of Organic Chemistry and Biochemistry

11. Other

Literature:	G. Odian, *Principles of Polymerization*, Wiley Interscience. S. Koltzenburg, M. Maskos, O. Nuyken, *Polymere*, Springer Spektrum. Further recommended literature will be announced in the courses.

Inorganic Materials Module No./ Code: MCh 20 WP 10	UNIVERSITÄT BONN

1. Contents and Qualification Objectives	
Contents	**Basics of inorganic materials:** metals, semiconductors, dielectric solids, ceramics, glass, nanomaterials; relation between structure, chemical bonding, and properties; electronic structure of solids, thermodynamics of heterogeneous equilibria (solid-liquid-gaseous); solids with homogeneity range; electronic structure of ions of the d- and f-block. **Synthesis of solids:** solid state reactions, sol-gel synthesis, hydrothermal synthesis, crystallization from the gas phase (solid-gas reactions, chemical vapor transport), microwave assisted syntheses, synthesis of thermodynamically metastable solids, ways to synthesize nano-materials. **Characterization:** diffraction methods; optical spectroscopy (UV/VIS, IR, Raman); electron spectroscopy (EDX, EELS), nuclear magnetic resonance; magnetic measurements; optical characterization (optical microscopy, electron microscopy). **Materials properties/application:** solid ionic conductors and their application in fuel cells; functional ceramics with dielectric and magnetic properties (piezoelectrics, spintronics, etc.) and their application in electronic devices; heterogeneous catalysis (e.g. Fischer-Tropsch, Haber-Bosch, three-way catalyst); optical properties and application of solids as color and luminescent pigments. **Lab course:** “demanding" solid state syntheses (air and/or moisture sensitive compounds, well-defined reaction atmosphere, metastable solids): • Chemical vapor transport experiment incl. computation of heterogeneous equilibria and transport rate • Solid state reactions followed by phase analysis of products by diffraction methods and spatially resolved analysis using the electron microscope • Sol-gel synthesis of thin films on a substrate and determination of their crystal structure and micro structure as a function of temperature of synthesis • Synthesis of nano-scale crystals and their characterization by diffraction and electron microscopic methods
Qualification Targets	• Acquiring advanced knowledge of synthesis, characterization, structure, properties and applications of inorganic materials • Synthesis and characterization of inorganic materials • Ability to present scientific results appropriately in oral and written form

2. Course Format						
	Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr] (On-Site/ SLT)
	L	Inorganic materials	en.	20	4	120 (60 / 60)
	S	Seminar for the lecture	en.	20	1	40 (15 / 25)
	LC	Experiments on lecture topics	en.	2	4	140 (60 / 80)

3. Module Prerequisites	
Required	Passed module MCh 20 1.1
Recommended	

4. Module Application			
	Degree Program/ Component	Compulsory/ Elective	Program-Related Semester
	MSc Chemistry	Elective	2 or 3

5. Requirements for ECTS Credit Points		**6. ECTS CP**
Study Achievement(s)	Lab reports	**10**
Examinations and Examination Language	Written examination; en.	

7. Cycle		**8. Workload**	**9. Duration**
Winter semester ☒ Summer semester ☐	Winter and summer semester ☐	**300 hr**	**1 semester**

10. Module Organization	
Instructor	Prof. Dr. R. Glaum, Prof. Dr. J. Beck, Dr. W. Assenmacher, Dr. J. Daniels
Module Coordinator	Prof. Dr. R. Glaum
Organizational Unit Offering the Module	Department of Chemistry (FMNS), Institute for Inorganic Chemistry

11. Other	
Literature:	A. R. West, *Solid State Chemistry and Its Applications*, Wiley. L. E. Smart, E. A. Moore, *Solid State Chemistry*, Yonsei Univ. Books. C. E. Housecroft, A. G. Sharpe, *Inorganic Chemistry*, Pearson. B. N. Figgis, M. A. Hitchman, *Ligand field theory and its applications*, Wiley-VCH.

Biophysical Chemistry Module No./ Code: MCh 20 WP 11	UNIVERSITÄT BONN

1. Contents and Qualification Objectives

Contents	**Molecules of the Cell I:** water, ions, lipids, nucleic acids, proteins, saccharides. **Structure of Cells:** Prokaryotes and eukaryotes. **Molecules of the Cell II – Proteins:** physical interactions in proteins (electrostatics incl. Debye-Hückel theory, dipolar interactions, steric repulsion, hydrogen bonding, hydrophobic effect), simulation of protein structure and dynamics (MD-simulation), protein folding, specific binding/molecular recognition, molecular crowding (statistical model, impact on binding constants, structural changes). **Molecules of the Cell III – RNA:** structure and function of ribozymes: Mechanism and impact of metal ions. structure and function of riboswitches: switching mechanisms and impact on gene expression. Small RNAs. **Molecules of the Cell IV – Biomembranes:** hydrophobic effect, self-aggregation and fluid-mosaic-model, membrane potentials (diffusion potential, electro-diffusion equation, Donnan potential, Goldmann equation), molecular foundation of the selectivity of ion channels, conductibility of active membranes. **Methods of Biophysical Chemistry:** modern thermodynamical methods, modern microscopic and spectroscopic techniques, crystal structure analysis, key experiments in biophysical chemistry, exemplary application of the concepts presented in the lectures. **Lab Course in Biophysical Chemistry:** optical and functional microscopy, thermodynamic techniques, analysis of biomacromolecules using spectroscopic methods.
Qualification Targets	• In-depth knowledge of biophysical chemistry • Understanding life processes in physicochemical terms • Application of the knowledge gained to the solution of theoretical and practical problems • Independent implementation and evaluation of experiments using the methods of biophysical chemistry

2. Course Format

	Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr] (On-Site/ SLT)
	L	Biophysical chemistry	en.	20	2	60 (30 / 30)
	S	Seminar for the lecture	en.	20	2	90 (30 / 60)
	LC	Experiments on lecture topics	en.	2	4	150 (60 / 90)

3. Module Prerequisites

Required	Passed module MCh 20 1.3
Recommended	

4. Module Application			
	Degree Program/ Component	Compulsory/ Elective	Program-Related Semester
	MSc Chemistry	Elective	2 or 3

5. Requirements for ECTS Credit Points		**6. ECTS CP**
Study Achievement(s)	Lab reports and seminar presentation	**10**
Examinations and Examination Language	Final oral examination; en.	

7. Cycle		**8. Workload**	**9. Duration**
Winter semester ☒ Summer semester ☐	Winter and summer semester ☐	**300 hr**	**1 semester**

10. Module Organization	
Instructor	Prof. Dr. U. Kubitscheck, Prof. Dr. R. Merkel
Module Coordinator	Prof. Dr. U. Kubitscheck
Organizational Unit Offering the Module	Department of Chemistry (FMNS), Institute of Physical and Theoretical Chemistry

11. Other	
Literature:	J. Kuriyan, B. Konforti, D. Wemmer, *The Molecules of Life: Physical Principles and Cellular Dynamics*, Garland Pub. D. Klostermeier, M.G. Ruldoph, *Biophysical Chemistry*, Apple Academic Press Inc. Additional current literature will be provided

Theoretical Methods for Condensed Matter Module No./ Code: MCh 20 WP 12	
1. Contents and Qualification Objectives	
Contents	Non-covalent interactions (NCI) between atoms and molecules (also misleadingly referred to as “non bonding” or “weak” interactions) are essential for the formation of condensed matter (e.g. liquids or molecular crystals). An important feature differentiating this from covalent bonds is the additive and thus cumulative character of the non-covalent interactions. Thus individually small contributions can add up to high overall binding energies in medium-sized systems. Modern quantum chemical methods of wave-function theory or density-functional theory are able to quantitatively describe these NCIs and thus open up a theoretical approach to a large number of material properties. In the first part of the course, the theoretical fundamentals of the NCIs are presented, and practical aspects of their calculation are discussed for various systems and illustrated in the practical course for typical examples. NCIs are particularly important in liquids and for solvent effects, which are preferably treated with molecular dynamics simulations. Concrete concepts for the description of the NCIs in such simulations (meaning from force fields to "on the fly" calculated potentials) are dealt with in the second part. In the course of such calculations, the multiplicity of data that is contained in the so-called trajectories must be analyzed. In the practical course, liquid systems and the corresponding work steps are to be understood based on specific examples. The quantum-chemical description of crystalline solids and their surfaces differs fundamentally from the treatment of molecular systems due to the translation symmetry. Both the Hamilton operator and the wave function must fulfill periodic boundary conditions. As a consequence, there are in principle infinite interaction integrals, and the total wave function would have to be composed of infinite crystal orbitals. In the third part of the lecture, the theoretical foundations of the approaches are presented that solve these problems. The concept of reciprocal space is introduced for this purpose. The number of orbitals can then be reduced to a finite number by selecting specific points in the irreducible Brillouin-zone. As basic functions, Bloch functions are used either from plane waves or atom-centered functions, resulting in different approaches for the approximate calculation of the finite grid sums. In the practical course, the students will be using the crystal orbital program CRYSTAL to treat selected solids and surfaces. Atomization energies, lattice parameters, band structures as well as adsorption structures and energies are calculated.
Qualification Targets	• Advanced knowledge of quantum chemical methods to investigate crystals and liquids • Practical application and interpretation of quantum chemical calculations of condensed matter • Preparation for own work in the field of theoretical chemistry of condensed matter • Learning competence • Methodological competence • Self-competence

2. Course Format						
	Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr] (On-Site/ SLT)
	L/S	Theoretical chemistry of solid state materials	en.	20	3	120 (45 / 75)
	LC	Practical exercises for the lecture topics	en.	20	6	180 (90 / 90)

3. Module Prerequisites	
Required	Passed module MCh 20 1.4
Recommended	

4. Module Application			
	Degree Program/ Component	Compulsory/ Elective	Program-Related Semester
	MSc Chemistry	Elective	2 or 3

5. Requirements for ECTS Credit Points		6. ECTS CP
Study Achievement(s)	Lab reports	**10**
Examinations and Examination Language	Final oral examination; en.	

7. Cycle		8. Workload	9. Duration
Winter semester ☒ Summer semester ☐	Winter and summer semester ☐	**300 hr**	**1 semester**

10. Module Organization	
Instructor	Prof. Dr. T. Bredow, Prof. Dr. B. Kirchner, Prof. Dr. S. Grimme
Module Coordinator	Prof. Dr. T. Bredow
Organizational Unit Offering the Module	Department of Chemistry (FMNS), Institute of Physical and Theoretical Chemistry

11. Other	
Literature:	A. J. Stone, *The Theory of Intermolecular Forces*, Clarendon Press. R. Hoffmann, R. Dronskowski, *Computational Chemistry of Solid State Materials: A Guide for Material Scientists, Chemists, Physicists and Others,* Wiley-VCH. A. R. Leach, *Molecular Modeling*, Prentice Hall. C. Kittel, *Einführung in die Festkörperphysik*, Oldenbourg.

Synthesis and Retrosynthesis Module No./ Code: MCh 20 WP 13	UNIVERSITÄT BONN

1. Contents and Qualification Objectives

Contents	**Theory:** • Retrosynthesis and synthetic strategies • Application of modern synthetic methods for the synthesis of complex functional compounds • Discussion of complex syntheses of natural products and drugs • Selected modern concepts (i.e. symmetry, intramolecularization, tandem processes, multi component reactions, biomimetic synthesis) • Application of modern NMR methods for determining the 2D and 3D structure of functional compounds **Lab course:** • Selected aspects of laboratory practice for organic chemistry: Reaction control, chromatography, GC, HPLC, reaction optimization • 2D and 3D determination of complex organic compounds by NMR spectroscopy • Interactive formulation of retrosynthesis and synthetic plans of complex functional compounds
Qualification Targets	• Detailed knowledge of modern synthetic procedures • Understanding and evaluation of complex target syntheses with a focus on natural products • Advanced laboratory practices • Advanced knowledge of NMR spectroscopic techniques for 2D and 3D structural assignment • Written documentation of scientific results • Efficient time management • Information management • Organizational skills • Further training of experimental skills • Further training of observation skills • Development of problem solving skills • Development of analytical skills, e.g. application of concepts of organic chemistry for an independent design of synthetic routes for complex functional compounds • Further development of decision making skills • Further training of accuracy and responsibility • Further development of communication skills • Further training of (self-) critical assessment

2. Course Format

	Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr] (On-Site/ SLT)
	L/S	Organic synthesis and retrosynthesis	en.	30	6	180 (90 / 90)
	LC	Experiments on lecture/seminar topics	en.	1–5	3	120 (45 / 75)

3. Module Prerequisites				
Required	Passed module MCh 20 1.2			
Recommended				
4. Module Application				
	Degree Program/ Component		Compulsory/ Elective	Program-Related Semester
	MSc Chemistry		Elective	2 or 3
5. Requirements for ECTS Credit Points				**6. ECTS CP**
Study Achievement(s)	Lab reports and seminar presentation			**10**
Examinations and Examination Language	Written examination; en.			
7. Cycle		**8. Workload**	**9. Duration**	
Winter semester ☒ Summer semester ☐	Winter and summer semester ☐	**300 hr**	**1 semester**	
10. Module Organization				
Instructor	Prof. Dr. D. Menche			
Module Coordinator	Prof. Dr. D. Menche			
Organizational Unit Offering the Module	Department of Chemistry (FMNS), Kekulé Institute of Organic Chemistry and Biochemistry			
11. Other				
Literature:	Recommended literature will be announced in the courses.			

Modern Methods to Elucidate Structure-Function-Relationships in Biomacromolecules

Module No./ Code: MCh 20 WP 14

1. Contents and Qualification Objectives

Contents	**Lecture:**
	• Basics of biochemistry
	• Structural biology: relationship between structure and function
	• Theoretical background of macromolecular crystallography
	• Solving the crystal structure of a protein
	• Cryo EM
	• Bio EPR
	• Bio NMR
	• FRET, SAXS
	• Worked examples of how to solve complex problems in structural biology:
	  o Crispr/Cas9
	  o Injection systems
	  o Ion channels and transporters
	  o Natural product synthesis
	  o Molecular rulers
	• "Emerging techniques": free electron laser
	Lab course:
	• Protein expression and purification
	• Activity assay
	• Crystallization
	• Solving the crystal structure of a protein

Qualification Targets	• Basics of biochemistry with a focus on structural biology • Theoretical background of structure determination with various methods • Protein expression, purification and characterization • Processing of diffraction data, solving macromolecular structures with crystallographic methods • Apply acquired knowledge to new problems • Solving complex problems by combining suitable scientific methods • Awareness of limitations of scientific methods • Responsible working behavior in a scientific laboratory • Good laboratory practice • Proper documentation of scientific results • Critical assessment of scientific results

2. Course Format

	Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr] (On-Site/ SLT)
	L/S	Analytical methods in structural biology	en.	30	3	120 (45 / 75)
	LC	Experiments on lecture/seminar topics	en.	2	6	180 (90 / 90)

<table>
<tr><td colspan="5">3. Module Prerequisites</td></tr>
<tr><td>Required</td><td colspan="4">Passed module MCh 20 1.3</td></tr>
<tr><td>Recommended</td><td colspan="4"></td></tr>
<tr><td colspan="5">4. Module Application</td></tr>
<tr><td rowspan="2"></td><td colspan="2">Degree Program/ Component</td><td>Compulsory/ Elective</td><td>Program-Related Semester</td></tr>
<tr><td colspan="2">MSc Chemistry</td><td>Elective</td><td>2 or 3</td></tr>
<tr><td colspan="4">5. Requirements for ECTS Credit Points</td><td>6. ECTS CP</td></tr>
<tr><td>Study Achievement(s)</td><td colspan="3">Lab reports</td><td rowspan="2">10</td></tr>
<tr><td>Examinations and Examination Language</td><td colspan="3">Final oral examination; en.</td></tr>
<tr><td colspan="2">7. Cycle</td><td>8. Workload</td><td colspan="2">9. Duration</td></tr>
<tr><td>Winter semester ☒
Summer semester ☐</td><td>Winter and summer semester ☐</td><td>300 hr</td><td colspan="2">1 semester</td></tr>
<tr><td colspan="5">10. Module Organization</td></tr>
<tr><td>Instructor</td><td colspan="4">PD Dr. G. Hagelüken</td></tr>
<tr><td>Module Coordinator</td><td colspan="4">PD Dr. G. Hagelüken</td></tr>
<tr><td>Organizational Unit Offering the Module</td><td colspan="4">Department of Chemistry (FMNS), Institute of Physical and Theoretical Chemistry</td></tr>
<tr><td colspan="5">11. Other</td></tr>
<tr><td>Literature:</td><td colspan="4">B. Rupp, Biomolecular Crystallography: Principles, Practice, and Application to Structural Biology, Garland Science.
J. W. Engels, F. Lottspeich, Bioanalytik, Springer Spektrum.</td></tr>
</table>

Natural Product Chemistry

Module No./ Code: MCh 20 WP 15

UNIVERSITÄT BONN

1. Contents and Qualification Objectives

<table>
<tr><td>Contents</td><td>Theory:
• Historical background
• Terms and definitions
• Classes of natural products:
  o Fatty acids, polyketides and prostaglandins
  o Terpenes including steroids and carotenoids
  o Alkaloids
  o Amino acids, ribosomal and non-ribosomal peptides
• Methods of structure elucidation:
  o NMR spectroscopy including 2D NMR techniques
  o Elucidation of relative configuration
  o Elucidation of absolute configuration
  o GC/MS and HPLC/MS including HRMS techniques
• Biosynthesis of natural products:
  o Classical methods (feeding of isotopically labeled precursors)
  o Modern methods (genetics, molecular and structural biology)
  o Gene regulation
  o Bioinformatics in natural product chemistry
• Drugs:
  o Important classes (antibiotics, cytostatic and virustatic compounds, etc.)
  o Structure activity relationship, drug design
Lab course:
Synthesis and analysis, e. g. preparation of isotopically labeled precursors for feeding experiments, synthesis of reference compounds for structure elucidation, isolation and structure elucidation by NMR of small natural products, GC/MS analysis of complex mixtures of natural products, gene cloning and purification of recombinant enzymes for biosynthetic studies.</td></tr>
<tr><td>Qualification Targets</td><td>• Basic knowledge of natural product chemistry
• Knowledge of structure elucidation, synthesis and biosynthesis of natural products
• Biological function of natural products, drugs
• Isolation (chromatographic purification) of natural products
• Structure elucidation by spectroscopic methods
• Elucidation of the biosynthesis of natural products by isotopic labeling experiments, genetic and enzymologic approaches</td></tr>
</table>

2. Course Format

	Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr] (On-Site/ SLT)
	L/S	Natural product chemistry	en.	30	4	120 (60 / 60)
	LC	Experiments on lecture/seminar topics	en.	1–3	6	180 (90 / 90)

3. Module Prerequisites			
Required	Passed module MCh 20 1.2		
Recommended	Participation in working group seminar for in-depth discussion of natural product biosynthesis problems		
4. Module Application			
	Degree Program/ Component	Compulsory/ Elective	Program-Related Semester
	MSc Chemistry	Elective	2 or 3
5. Requirements for ECTS Credit Points			**6. ECTS CP**
Study Achievement(s)	Lab report		**10**
Examinations and Examination Language	Final oral examination; en.		
7. Cycle		**8. Workload**	**9. Duration**
Winter semester ☒ Summer semester ☐	Winter and summer semester ☐	**300 hr**	**1 semester**
10. Module Organization			
Instructor	Prof. Dr. J. Dickschat		
Module Coordinator	Prof. Dr. J. Dickschat		
Organizational Unit Offering the Module	Department of Chemistry (FMNS), Kekulé Institute of Organic Chemistry and Biochemistry		
11. Other			
Literature:	P. M. Dewick, *Medicinal Natural Products*, Wiley. C. T. Walsh, Y. Tang, *Natural Product Biosynthesis*, Royal Society of Chemistry.		

Physical Concepts of Condensed Matter Science

Module No./ Code: MCh 20 WP 16

UNIVERSITÄT BONN

1. Contents and Qualification Objectives	
Contents	The topics covered in this module encompass the fundamental physical concepts and mathematical models that underlie condensed matter science: • The solid as a continuum • Elastic, thermal, electric and magnetic properties • The solid as crystalline and amorphous arrangements of atoms • Quasi-two- and quasi-one-dimensional materials • Phases, phase transitions and critical phenomena in condensed matter • Symmetry and its influence on the structural, electronic and magnetic phases and on the physical properties of solids • Transport in solids • Defects in solids • Energy landscape and structure prediction of solids • Many-particle aspects and quasi-particles and elementary excitations of solids • Interaction of solids with external probes, such as electromagnetic fields, temperature, and pressure This is complemented by the application of these concepts to modern crystalline, amorphous, quasi-two-dimensional and quasi-one-dimensional materials, such as high-Tc superconductors, graphene, liquid crystals, layered materials, or topological insulators. While all topics will be addressed in every cycle, the focus in the second term will partly vary, in order to allow an in-depth analysis of specific fundamental concepts.
Qualification Targets	This module will provide students insights into the classical and modern physical concepts of condensed matter science and their application to modern materials. The student will become familiar with basic and advanced atomistic and phenomenological mathematical models for the description of physical properties of solids. These include both crystalline and amorphous materials, and quasi-two- and quasi-one-dimensional materials. The student will acquire the conceptual knowledge needed to model modern solid materials and their physical properties, and to understand current research in condensed matter science. The following key competences will be addressed: • Ability to apply the acquired concepts to model systems • Ability to judge the level and appropriateness of mathematical models of solid materials • Ability to relate fundamental physical concepts (for instance: symmetry considerations) to the physical properties of materials • Ability to understand, interpret and communicate current research in condensed matter science • Ability to deepen conceptual understanding by independent study of the literature.

2. Course Format						
	Course Type	Topic	Language of Instruction	Group Size	Course Units per Week	Workload [hr]
	L	Physical concepts and mathematical models of condensed matter science	en.	20	2x2	2x60 (2x30 / 2x30)
	S	Seminar on lecture topics	en.	20	2x2	2x90 (2x30 / 2x60)

3. Module Prerequisites	
Required	None
Recommended	Passed modules MCh 20 1.1, MCh 20 1.3 and MCh 20 1.4

4. Module Application			
	Degree Program/ Component	Compulsory/ Elective	Program-Related Semester
	MSc Chemistry	Elective	1 and 2[1] or 2 and 3[2] or 3 and 4[1]

5. Requirements for ECTS Credit Points		6. ECTS CP
Study Achievement(s)	None	10
Examinations and Examination Language	Written examination; en.	

7. Cycle		8. Workload	9. Duration
Winter semester ☐ Summer semester ☐	Winter and summer semester ☒	**300 hr**	**2 semester**

10. Module Organization	
Instructor	Apl. Prof. Dr. J. C. Schön
Module Coordinator	Apl. Prof. Dr. J. C. Schön
Organizational Unit Offering the Module	Department of Chemistry (FMNS), Institute for Inorganic Chemistry

11. Other	
Literature:	N. W. Ashcroft, N. D. Mermin, *Solid State Physics*, Saunders College Publ. R. Balian, *From Microphysics to Macrophysics*, Springer. P. M. Chaikin, T. C. Lubensky, *Principles of Condensed Matter Physics*, Cambridge Univ. Press. S. R. Elliott, *The Physics and Chemistry of Solids*, Wiley. B. Lautrup, *Physics of Continuous Matter: Exotic and Everyday Phenomena in the Macroscopic World*, Inst. of Physics Bristol. C. Kittel, *Einführung in die Festkörperphysik*, Oldenbourg. K.-H. Hellwege, *Einführung in die Festkörperphysik*, Springer. C. Kittel, *Quantum Theory of Solids*, Wiley. J. R. Christman, *Festkörperphysik*, Oldenbourg. H. Ibach, H. Lüth, *Festkörperphysik: Einführung in die Grundlagen*, Springer. R. K. Pathria, P. D. Beale, *Statistical Mechanics*, Elsevier BH; or: R. K. Pathria *Statistical Mechanics*, Pergamon Press. M. Plischke, B. Bergersen, *Equilibrium Statistical Physics*, World Scientific. J. D. Jackson, *Classical Electrodynamics*, Wiley. E. M. Purcell, *Berkeley Physics Course Volume 2 – Electricity and Magnetism*, McGraw-Hill. H. Goldstein, C. P. Poole, J. L. Safko, *Klassische Mechanik*, Wiley-VCH. D. S. Lemons, *A Student's Guide to Dimensional Analysis*, Cambridge University Press. L. D. Landau, E. M. Lifschitz, *Lehrbuch der Theoretischen Physik III: Quantenmechanik*, Akademie Verlag Berlin.
Notes:	This lecture is open to all participants from the Faculty of Mathematics and Natural Sciences. Please note the order of the two lecture parts: The module begins each summer semester. The content of the 2nd part in the winter semester builds on the 1st part taken in the summer semester. This results in the following program-related semesters for the module: [1]: If program starts in the summer semester [2]: If program starts in the winter semester

Magnetic Resonance Spectroscopy Module No./ Code: MCh 20 WP 17	UNIVERSITÄT BONN

1. Contents and Qualification Objectives	
Contents	**Lecture:** • The spin • Interaction between spin and magnetic field/electromagnetic radiation • Bloch equations • Spectrometer setup: sources, wave guides, resonators • T_1/T_2 relaxation and line shapes • Liouville/von Neumann equation • Spin-Hamiltonian for NMR and EPR • Pulses, FIDs and echoes • Pulse sequences and spin dynamics • Coherence transfer pathways and density matrix formalism **Exercise:** • Applications of Magnetic Resonance Theory • Calculation of spin dynamics • Transformations **Seminar:** Independently working out a topic from magnetic resonance spectroscopy and presenting the topic in the form of a 30 minute lecture followed by a discussion. **Lab course:** • Pulses, FIDs and echoes • Phase cycles • Relaxation measurements • Transient nutation
Qualification Targets	• Basic knowledge of spin physics • Basic knowledge of EPR/NMR theory • Basic understanding of the relationship between pulse sequence and spin dynamics • Application of the methods and concepts learned to questions of magnetic resonance spectroscopy

2. Course Format

	Course Type	Topic	Language of Instruction	Group Size	Cours e Units per Week	Workload [hr] (On-Site/ SLT)
	L	Magnetic Resonance Theory	en.	25	2	90 (30 / 60)
	S	Seminar presentation on a magnetic resonance spectroscopy topic	en.	25	2	90 (30 / 60)
	E	Applications of Magnetic Resonance Theory	en.	25	2	60 (30 / 60)
	LC	Experiments on magnetic resonance spectroscopy	en.	25	2	60 (30 / 60)

3. Module Prerequisites			
Required	Passed module MCh 20 1.3		
Recommended			
4. Module Application			
	Degree Program/ Component	Compulsory/ Elective	Program-Related Semester
	MSc Chemistry	Elective	2 or 3
5. Requirements for ECTS Credit Points			**6. ECTS CP**
Study Achievement(s)	50% of the achievable credits are for the exercises and lab reports		**10**
Examinations and Examination Language	Final oral examination; en.		
7. Cycle		**8. Workload**	**9. Duration**
Winter semester ☐ Summer semester ☒	Winter and summer semester ☐	**300 hr**	**1 semester**
10. Module Organization			
Instructor	Prof. Dr. O. Schiemann		
Module Coordinator	Prof. Dr. O. Schiemann		
Organizational Unit Offering the Module	Department of Chemistry (FMNS), Institute of Physical and Theoretical Chemistry		
11. Other			
Literature:	M. H. Levitt, *Spin Dynamic*, GB Wiley. A. Schweiger, G. Jeschke, *Principles of Pulse Electron Paramagnetic Resonance*, Oxford University Press.		