Import module

[E1.4]	EPR Spectroscopy	Compulsory elective module	7 - 10 CP (total) = 210 - 300 h		4 - 7 SWS
			Contact hours 4-7 SWS / 60-105 h	Independent study 150 - 195 h	

Content

Lecture: Quantum mechanical fundamentals of EPR spectroscopy, spin-Hamilton operators, magnetic dipole interactions, hyperfine interactions, QM fundamentals of G and zero-field tensors, basic experiments in EPR spectroscopy (cw-EPR, pulse EPR, relaxation times, hyperfine spectroscopy, dipolar spectroscopy), examples of applications of EPR spectroscopy from materials science, analytics, structural investigations of macromolecular systems, and EPR spectroscopy in electron transfer reactions in catalysis and photovoltaics.

Practical course: (optional) Cw-EPR experiments for the characterization of organic radical compounds, oxidation/reduction behavior and kinetics, cw-EPR experiments for the quantitative determination of radical concentrations in solutions, introduction to basic pulse EPR experiments (Hahn-Echo, Inversion Recovery Experiment) to determine relaxation times. Introduction to simulation software for determining hyperfine couplings in liquid solution and G-tensors in solid samples. Comparison with DFT calculations.

Seminar: (optional) Presentation on a current research publication in the field of magnetic resonance spectroscopy, selection of a suitable publication, literature research, development of the topic in interaction with one of the lecturers on magnetic resonance, lecture in the seminar, discussion of the presented method and the knowledge gained from this also in the context of the other seminar lectures/methods.

The courses Lecture Theory of electron paramagnetic resonance spectroscopy (compulsory) as well as another course Practical course / Seminar (CEM) must be attended.
The seminar is part of the modules Liquid NMR spectroscopy, EPR spectroscopy and solid state NMR spectroscopy. It can only be scored once.

Learning outcomes and skills

Quantum mechanical understanding of spin systems (energy eigenvalues in the magnetic field and temporal development under/after coherent excitation pulses, magnetic interaction between unpaired electron spins and with nuclear spins, spin-orbit coupling of the magnetic moment of the unpaired electron), knowledge of the fundamental experiments on determination of these interactions in liquid solutions and solid samples. Qualitative understanding of spin relaxation times and methods of determination. Insights into areas of application of EPR spectroscopy from chemical and materials science analysis to applications in catalysis, structural biology and photovoltaics.

Admissions requirements/Conditions for participation in the module/courses

Practical course and seminar: Expert discussion on the lecture *Theory of EPR spectroscopy*

Recommended prior knowledge

None

Organizational details

Import module, the registration and cancellation periods of the regulations for the Master's degree in chemistry apply. (An examination date for the expert discussion must be agreed with the examiner.)

Module allocation (degree programme/faculty)	Master Chemistry / FB14
Module transferrable to other degree programmes	Master Bioinformatics / FB12, Bachelor Biophysics / FB13, Master Biophysics / FB13, Master Physics / FB13, Master Biochemistry / FB14
Module offered	- Lecture: winter semester - Practical course: summer semester - Seminar: every semester
Duration	2 semesters
Module coordinator	Prof. Prisner
Course requirements for credits	
Participation record	- Seminar & practical course: regular and active participation
Coursework	- Lecture: Expert discussion (30 min.) - Practical course: Processing and protocols of the practical course experiments - Seminar: Paper presentation (20 min., handout)
Forms of teaching / learning	Lecture, practical course, seminar
Language teaching and instruction	English
Module assessment	**Form / duration / content, if applicable**
Final module assessment	None
Cumulative module assessment consisting of	
Composition of the module grade for cumulative module assessment	

		Mode of teaching / study	Semester hours per week	Semester CP			
				1	2	3	4
	Compulsory: Theory of electron paramagnetic resonance spectroscopy	L	2	4			
	CEM: Practical course in electron paramagnetic resonance spectroscopy	P	3		3		
	CEM: Modern applications of MR spectroscopy	S	2	3			
	TOTAL		4-7	7-10			