COURSE UNIT (MODULE) DESCRIPTION

Course unit (module) title	Code
X-ray Diffraction Analysis	

Lecturer(s)	Department(s) where the course unit (module) is delivered
Coordinator: Ramūnas Skaudžius **Other(s):**	Faculty of Chemistry and Geosciences, Institute of Chemistry Naugardukas str. 24, LT-03225 Vilnius

Study cycle	Type of the course unit (module)
Second	Optional

Mode of delivery	Period when the course unit (module) is delivered	Language(s) of instruction
Face to face	1st semester	English and Lithuanian

Requirements for students	
Prerequisites: main courses of chemistry or nanomaterial chemistry bachelor programs: general chemistry, inorganic chemistry, chemistry of crystals and etc.	**Additional requirements (if any):** To have a PC for seminars.

Course (module) volume in credits	Total student's workload	Contact hours	Self-study hours
5	135	64	71

Purpose of the course unit (module): programme competences to be developed		
After successful completion of this course student will know the theory of x-ray diffraction and will apply it for the qualitative and quantitative analysis by Rietveld or Le Bail fitting methods.		
Learning outcomes of the course unit (module)	**Teaching and learning methods**	**Assessment methods**
Student will able to explain theoretical background of X-Ray diffraction (XRD) measurements;	Lectures with demonstrations how to use the program for XRD data; Individual literature study.	Final exam (written and oral open answer questions).
Student will able to prepare samples for XRD analysis and choose proper conditions for XRD measurement;	Laboratory work; Individual literature study.	All laboratory works must be done, laboratory reports must be compiled and defended.
Student will able to analyze data by Le Bail Fitting and Rietveld methods;	Seminars and group tutorials how to use the program for XRD data analysis; Individual literature study.	Individual data analysis by presented requirements.
Student will able to present experimental results graphically.	Seminars and group tutorials how to use the program for XRD data analysis; Presentation.	Individual data analysis.

Content: breakdown of the topics	Contact hours					Total contact hours	Self-study hours	Self-study work: time and assignments
	Lectures	Seminars	Exercises	Laboratory work	Internship/work placement			Assignments
1. Introduction. Course objectives.	1	1				2	**1**	To install required programs.
2. The discovery of X-ray and the most important historic scientific achievements. X-ray nature. Advantages and outs of X-ray diffraction (XRD) analysis. Comparison of neutron and X-ray diffraction.	2	1				3	**6**	Textbook reading. Problem solving. Test programs.
3. The X-ray sources. The unit cell. Miller indices. Diffractometer cameras and geometry.	2	2				4	**6**	Textbook reading. Literature search. Problem solving. Convert XRD patterns to different type of files.
4. Braggs' law. Detectors. "Anatomy" of XRD pattern. Sample preparation.	2	2		4		8	**10**	Textbook reading. Preparation of laboratory work reports. XRD pattern analysis by presented requirements.
5. Conditions for X-ray measurements. Qualitative analysis.	2	2		4		8	**10**	Textbook reading. Preparation of laboratory work reports. XRD pattern analysis by presented requirements.
6. Le Bail fitting method.	1	8		4		13	**10**	Textbook reading. Preparation of laboratory work reports. XRD pattern analysis by presented requirements.
7. Rietveld method.	1	8		4		13	**10**	Textbook reading. Preparation of laboratory work reports. XRD pattern analysis by presented requirements.
8. Data analysis after Rietveld and presenting results.	1	2				3	**6**	Textbook reading. Individual sample analysis.
9. Defects. Microstrains. Crystallite size.	2	2				4	**6**	
10. Quantitative analysis by Rietveld method and other	2	4				6	**6**	Textbook reading. XRD pattern analysis by presented

various type of XRD analysis								requirements. Individual sample analysis.
Total	**16**	**32**		**16**		**64**	**71**	

Assessment strategy	Weight,%	Deadline	Assessment criteria
Laboratory work	Pass/Fail	October-December	One-to one conversation (understanding of theoretical background is tested). Safe work with instrument. Ability to get reliable results. Detailed criteria is presented during lectures. All laboratory works must be done, laboratory reports must be compiled and defended in one-to one conversation. In case of Fail, student must repeat the course next year.
Individual data analysis by presented requirements.	40%	December	Analyse individual XRD pattern by presented requirements. Evaluation of other students' data treatment by presented grading scheme during lectures.
Final exam	60%	January	Open questions (written and oral).

Author	Year of publication	Title	Issue of a periodical or volume of a publication	Publishing place and house or web link
Compulsory reading				
Cullity, B.D. and Stock, S.R.	2001	Elements of X-Ray Diffraction	Addison-Wesley	Physical Sciences Reading Room
Ermrich M. and Opper D.	2013	XRD for analyst	PANanalytical GmbH	https://imf.ucmerced.edu/sites/imf.ucmerced.edu/files/page/documents/x-ray_powder_diffraction.pdf
Optional reading				
Rodrigues-Carvajal J.	2000	An Introduction to the Program FullProf	-	https://www.psi.ch/sinq/dmc/ManualsEN/fullprof.pdf
Pynn R.	1990	Neutron Scattering – A primer	LANSCE	https://www.ncnr.nist.gov/summerschool/ss16/pdf/NeutronScatteringPrimer.pdf
Stahl K.	2008	Powder Diffraction and the Rietveld method	Lyngby	