Attachment No. 5 to Rector's ordinance No. 22/2020

DESCRIPTION OF THE COURSE OF STUDY

Course code	**0531-2CHEM-C11-K**	
Name of the course in	Polish	*Krystalografia*
	English	*Crystallography*

1. LOCATION OF THE COURSE OF STUDY WITHIN THE SYSTEM OF STUDIES

1.1. Field of study	**Chemistry**
1.2. Mode of study	**Full-time studies**
1.3. Level of study	**2st degree**
1.4. Profile of study*	**General academic**
1.5. Person/s preparing the course description	**Agnieszka Jabłońska-Wawrzycka, Professor**
1.6. Contact	**Agnieszka.Jablonska-Wawrzycka@ujk.edu.pl**

2. GENERAL CHARACTERISTICS OF THE COURSE OF STUDY

2.1. Language of instruction	**English**
2.2. Prerequisites*	**Fundamentals of Crystallography, Inorganic Chemistry, Physical Chemistry, Maths, Physics**

3. DETAILED CHARACTERISTICS OF THE COURSE OF STUDY

3.1. Form of classes		Lectures (15 hrs), Seminar (20 hrs), Laboratory classes (30 hrs)
3.2. Place of classes		Classes in the teaching room of the UJK
3.3. Form of assessment		Lecture – exam, Seminar - credit with grade, Laboratory classes – credit with grade
3.4. Teaching methods		Lecture - informative lecture, conversational lecture, description, Seminar - subject exercises, computer-aided learning, project, Laboratory - laboratory exercises, measurement, computer-aided learning;
3.5. Bibliography	**Required reading**	G. Zanotti, G. Gilli, H.L. Monaco, D. Viterbo, C. Giacovazzo, M. Catti, F. Scordari, Fundamentals of Crystallography, Oxford University Press, 1992. C. Giacovazzo, Fundamentals of Crystallography, 2nd Edition, IUCR, Oxford University Press, 2002. J. P. Glusker, K. N. Trueblood, Crystal Structure Analysis: a primer, Oxford University Press, 1972. M. M Woolfson, An Introduction to X-ray Crystallography, 2nd Edition, Cambridge University Press, 1997.
	Further reading	F. Hoffmann, Introduction to Crystallography, Springer, 2020.

4. OBJECTIVES, SYLLABUS CONTENT AND INTENDED LEARNING OUTCOMES

4.1. Course objectives ***(including form of classes)***

C1 - recall and extension of basic knowledge in the field of crystallography enabling the characterization of the crystalline state, determining the symmetry of the crystal, developing visual-spatial skills, (Lecture, Seminar)

C2 – getting acquainted with crystallographic databases containing structural data of organometallic and inorganic compounds as well as crystallographic literature and skillful use of it; (Seminar, Laboratory)

C3 – developing the ability to find relationships between the structure and properties of crystals; reading and understanding the symbolism of Schoenflies and Hermann-Mauguin (international) (Seminar)

C4 – familiarization with crystallographic databases and graphic programs for visualizing these data (Seminar)

4.2. Detailed syllabus ***(including form of classes)***

Lecture

1. Recall and extension of material regarding: simple structure, plane and spatial lattice, Miller Indices, belt relation, crystallographic systems, types of Bravais translational networks, point groups and its symbols, product of transformations, crystallographic systems, space groups, translational symmetry elements.
2. Diffraction phenomenon - equivalence of Laue and Bragg equations.
3. Reciprocal lattice.
4. X-ray structural analysis. Structure factor F. Phase problem. Patterson function. Indirect and direct methods. Systematic extinctions. Solution quality parameters.
5. Selected crystal growing methods.
6. Sources of information about the structure of solids.

Seminar

1. Indexing directions and network planes.
2. Solving problems using the belt equation.
3. Determining interplanar distances using quadratic equations.
4. Elements of symmetry in crystallographic systems.
5. Structural characterization of selected compounds based on scientific publications (Science Direct On Site Database (ICM), Elsevier collection, Springer). Crystallographic databases (CCDC). Crystallographica Acta Journals. Structural characterization of chemical compounds based on a published scientific article.
6. Types of graphic programs for the interpretation of crystallographic data. Standard bond lengths. Forms of presentation of X-ray measurement results: bond lengths, valence angles, torsion angles.
7. The relationship between the coordination number and the geometry of the coordination polyhedron.

Laboratory classes

1. Selected crystallization methods.
2. Microscopic observations of interesting crystal forms.
3. Indexing lattice lines and planes using a computer using the Krys 1 program.
4. Basics of diffractometry. Solving issues related to the scattering of X-ray radiation by various types of matter.
5. X-ray phase analysis in a single- and multi-phase system using the ICDD database and the XRAYAN program. Indication of diffractograms of highly symmetric phases using the logarithmic strip method. Determination of network parameters after indexing XRD powder diffractograms. Indexing of diffractograms of selected phases, using the DICVOL program.

4.3 Intended learning outcomes

Code	A student, who passed the course	Relation to learning outcomes
within the scope of **KNOWLEDGE:**		
W01	has theoretical knowledge in the field of indexing lattice lines and planes, belt relations, interplanar distance	CHEM2A_W05
W02	knows the concepts that help determine the symmetry of molecules and crystallographic systems and use it to obtain information about the tested substance	CHEM2A_W05
W03	has knowledge of the properties of obtaining and using X-rays in the study of solids	CHEM2A_W05
W04	knows the relationship between a crystal and its diffraction pattern and also has knowledge about methods of collecting structural data and ways of obtaining this data and their use to solve scientific problems	CHEM2A_W05
W05	has knowledge of types of graphic programs for the interpretation of crystallographic data	CHEM2A_W05
W06	knows the regulations and rules regarding occupational health and safety in the X-ray laboratory	CHEM2A_W05
within the scope of **ABILITIES:**		
U01	has the ability to index lattice lines and planes and use the Kryst1 program, solves calculations regarding the belt relationship, simple tasks related to interplanar distance and X-ray radiation properties	CHEM2A_U03
U02	uses the commonly accepted Hermann-Maugin symbolism used to determine the symmetry of crystals and their internal structure	CHEM2A_U03
U03	identifies substances and their crystalline phases based on polycrystalline diffractograms and available databases using the X-rayan program; can indicate powder diffractograms for crystallographic systems with high symmetry	CHEM2A_U03
U04	knows and uses selected crystallization methods	CHEM2A_U03
U05	is able to analyze selected, simple models of crystal structures and classify crystal structures according to the types of chemical interactions	CHEM2A_U03
within the scope of **SOCIAL COMPETENCE:**		
K01	is aware of the interdisciplinary nature of crystallography among other fields of science	CHEM2A_K01
K02	demonstrates an accepting attitude towards mathematical and IT methods within the scope of the subject	CHEM2A_K01
K03	is aware of the possibilities of practical use of diffraction data to identify the phases of polycrystalline substances	CHEM2A_K03
K04	is aware of the potential dangers associated with the use of X-ray radiation	CHEM2A_K03

4.4. Methods of assessment of the intended learning outcomes							
Teaching outcomes *(code)*	**Method of assessment (+/-)**						
	Exam oral		**Test**			**Project, report**	
	Form of classes		***Form of classes***			***Form of classes***	
	L	*S*	*L*	*S*	*Lab*	*S*	*Lab*
W01	+	—	+	—	—	—	—
W02	+	—	+	—	—	—	—
W03	+	—	+	—	+	—	—
W04	+	—	+	—	—	—	+
W05	—	—	—	+	—	+	—
W06	—	—	—	—	+	—	—
U01	—	—	—	+	+	—	—
U02	+	—	+	+	—	—	—
U03	—	—	+	—	+	—	+
U04	+	—	+	—	+	—	+
U05	+	—	+	—	—	+	—
K01	+	—	—	—	—	—	—
K02	—	—	—	+	+	—	—
K03	—	—	—	—	+	—	+
K04	—	—	—	—	+	—	—

4.5. Criteria of assessment of the intended learning outcomes		
Form of classes	**Grade**	**Criterion of assessment**
Lecture (L) * (including e-learning)	**3**	Exam oral, obtaining 51-60% of the total number of available points
	3,5	Exam oral, obtaining 61-70% of the total number of available points
	4	Exam oral, obtaining 71-80% of the total number of available points
	4,5	Exam oral, obtaining 81-90% of the total number of available points
	5	Exam oral, obtaining 91-100% of the total number of available points
Seminar (S) ** (including e-learning)	**3**	Credit with grade – obtaining 51-60% of the total number of points from partial tests
	3,5	Credit with grade – obtaining 61-70% of the total number of points from partial tests
	4	Credit with grade – obtaining 71-80% of the total number of points from partial tests
	4,5	Credit with grade – obtaining 81-90% of the total number of points from partial tests
	5	Credit with grade – obtaining 91-100% of the total number of points from partial tests
Laboratory (Lab) *** (including e-learning)	**3**	Credit with grade – obtaining 51-60% of the total number of points from partial tests and reports for completed exercises
	3,5	Credit with grade – obtaining 61-70% of the total number of points from partial tests and reports for completed exercises
	4	Credit with grade – obtaining 71-80% of the total number of points from partial tests and reports for completed exercises
	4,5	Credit with grade – obtaining 81-90% of the total number of points from partial tests and reports for completed exercises
	5	Credit with grade – obtaining 91-100% of the total number of points from partial tests and reports for completed exercises

* L – The condition for taking the exam is obtaining at least 50% of the points in two partial tests; A student who obtains more than 65% points is exempt from the exam oral; The student receives three exam questions and, after short preparation, provides answers.

** S – Student receives a pass based on the points obtained in partial tests as well as a completed project, the effects of which are presented in the form of a report.
*** Lab – Student receives credit on the basis of: grades obtained in partial tests and reports for completed exercises.

5. BALANCE OF ECTS CREDITS – STUDENT'S WORK INPUT

Category	Student's workload	
	Full-time studies	Extramural studies
NUMBER OF HOURS WITH THE DIRECT PARTICIPATION OF THE TEACHER /CONTACT HOURS/	***65***	
*Participation in lectures**	***15***	
*Participation in classes, seminars, laboratories**	***20+30***	
INDEPENDENT WORK OF THE STUDENT/NON-CONTACT HOURS/	***65***	
*Preparation for the lecture**	***5***	
*Preparation for the classes, seminars, laboratories**	***25***	
*Preparation for the exam/test**	***20***	
TOTAL NUMBER OF HOURS	***10***	
ECTS credits for the course of study	***5***	

delete as appropriate

Accepted for execution *(date and legible signatures of the teachers running the course in the given academic year)*

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