LEARNING MODULE DESCRIPTION (SYLLABUS)

X-RAY STRUCTURE ANALYSIS

I. **General information**

1. Module title

   X-ray structure analysis

2. Module code

   XRSA

3. Module type – compulsory or optional

   Compulsory

4. Programme title

   Chemistry

5. Cycle of studies (1st or 2nd cycle of studies or full master's programme)

   second cycle of studies

6. Year of studies

   first year

7. Terms in which taught (winter/summer term)

   winter

8. Type of classes and the number of contact hours

   15 hours lectures; 30 hours laboratories

9. Number of ECTS credits

   5

10. Name, surname, academic degree/title of the module lecturer/other teaching staff/ e-mail
    Maciej Kubicki, Professor dr. hab., mkubicki@amu.edu.pl

11. Language of classes

    English

II. **Detailed information**

1. Module aim (aims)

The aim of the course is to familiarise students with:

- Basic knowledge allowing experimental studies on internal structure of crystals
- The effects of diffraction of the radiation on the crystal lattice; the reciprocal lattice
- Basics of computational methods involved in the crystal structure determination
- Preparation of short reports on the experimental results

2. Pre-requisites in terms of knowledge, skills and social competences (where relevant)
   Basic knowledge of physics, physical chemistry and crystal chemistry

3. Module learning outcomes in terms of knowledge, skills and social competences and their reference to programme learning outcomes

Learning outcomes symbol*	Upon completion of the course, students will:	Reference to programme learning outcomes#

XRSA _01	**be able to characterize the crystalline state, to show and describe the symmetry of the external shape of the crystal**	CHE2_W01,CHE2_W04, CHE2_U06, CHE2_K01
XRSA _02	**know how to describe the crystal lattice, including Miller indices, and how to draw and read the symmetry elements of the space group**	CHE2_W02, CHE2_W04, CHE2_U05
XRSA _03	**know the basics of diffraction of X-rays including Laue's and Bragg's equations**	CHE2_W02, CHE2_W07, CHE2_W07, CHE2_U05
XRSA _04	**know how to calculate the structure factor and how to predict the systematical extinctions for given space group**	CHE2_W02, CHE2_W09, CHE2_W12, CHE2_U05
XRSA _05	**have the basic knowledge of the techniques of X-ray generation, the properties of X-rays and the safety regulations.**	CHE2_W07, CHE2_W09, CHE2_U07, CHE2_K03
XRSA _06	**understand the phase problem and know the methods of solving it.**	CHE2_W02, CHE2_W07, CHE2_U05
XRSA _07	**be able to plan the diffraction experiment, to choose the appropriate crystal**	CHE2_W07, CHE2_U02, CHE2_U06
XRSA _08	**have the skills allowing to interpret the results of X-ray structure determination**	CHE2_W01, CHE2_W04, CHE2_U01, CHE2_U02, CHE2_U05, CHE2_U07, CHE2_U14, CHE2_K01
XRSA _09	**be able to critically analyze the published results of the structural X-ray analysis and to retrieve such data from the databases**	CHE2_W01, CHE2_W04, CHE2_U02, CHE2_U05, CHE2_U07, CHE2_U10, CHE2_U14, CHE2_K02
XRSA_10	**be able to apply safety rules in laboratory work**	CHE2_W07, CHE2_U15, CHE2_K02, CHE2_K03, CHE2_K04

* module code, e.g. KHT_01 (KHT – module code in USOS; stands for Polish "Analiza Instrumentalna" /Analytcial Chemistry/)
# programme learning outcomes (e.g. K_W01, K_U01, …); first K stands for programme title symbol in Polish, W for "wiedza" (knowledge) in Polish, U – for "umiejętności" (skills) in Polish, K – for "kompetencje społeczne" (social competences) in Polish
01, 02… - learning outcome number

3. Learning content

Learning content symbol	Learning content description	Reference to module learning outcomes
TK_01	**Crystalline state, symmetry, point groups. History of crystallography**	XRSA _01
TK_02	**Crystal lattice, Miller indices, Bravais lattice, translational elements of symmetry, space groups**	XRSA _02
TK_03	**Diffraction, interference, Laue theory, Braggs theory**	XRSA _01, XRSA _02, XRSA _03, XRSA _06
TK_04	**Atomic scattering factor, structure factor, Friedel's law, Laue classes, systematic absences**	XRSA _02, XRSA _03, XRSA _04, XRSA _06
TK_05	**X-rays generation, tubes, synchrotron, properties of X-rays, monochromatization, absorption**	XRSA _05, XRSA _07, XRSA _08, XRSA _10
TK_06	**Policrystalline methods, identification of phases**	XRSA _01, XRSA _03, XRSA _06, XRSA _07, XRSA _08, XRSA _09
TK_07	**Phase problem, Patterson method, direct methods. Fourier maps**	XRSA _02, XRSA _03, XRSA _04, XRSA _06, XRSA _09
TK_08	**X-ray structure determination in practice: from crystal selection to structure refinement**	XRSA _01, XRSA _04, XRSA _06, XRSA _07, XRSA _08, XRSA _09, XRSA _10

TK_09	**Analysis of the results: coordinates, geometry, interactions. Graphical presentation**	XRSA _05, XRSA _07, XRSA _08, XRSA _09
TK_10	**Structural databases: CCDC, PDN etc.**	XRSA _05, XRSA _07, XRSA _08, XRSA _09

e.g. TK_01, TK_02, … (TK stands for "treści kształcenia" /learning content/ in Polish)
e.g. AINE_01– module code as in Table in II.3

4. Reading list

1) **C. Hammond, The basics of crystallography and diffraction, Oxford University Press (3rd ed.), 2009**

5.Information on where to find course materials

Course materials can be downloaded from the web-page of the Department of crystallography.

III. **Additional information**

1. Reference of learning outcomes and learning content to teaching and learning methods and assessment methods

Lecture topic are closely related to laboratory exercises. Lectures provide the background and extensions for the labs.

Symbol of module learning outcome*	Symbol of module learning content#	Methods of teaching and learning	Assessment methods of LO achievement&
XRSA _01	TK_01, TK_03, TK_06,TK_08	Lectures, laboratory work, laboratory reports	F- discussion, observation, correction of laboratory work; S - final exam; S- part-time exam
XRSA _02	TK_02, TK_03, TK_04, TK_07	Lectures, laboratory work, laboratory reports	F- discussion, observation, correction of laboratory work; S - final exam; S- part-time exam
XRSA _03	TK_03, TK_04, TK_06, TK_07	Lectures, laboratory work, laboratory reports	F- discussion, observation, correction of laboratory work; S - final exam; S- part-time exam
XRSA _04	TK_04, TK_07, TK_08	Lectures, laboratory work, laboratory reports	F- discussion, observation, correction of laboratory work; S - final exam; S- part-time exam
XRSA _05	TK_05, TK_09, TK_10	Lectures, laboratory work, laboratory reports	F- discussion, observation, correction of laboratory work; S - final exam; S- part-time exam
XRSA _06	TK_03, TK_04, TK_06, TK_07, TK_08	Lectures, laboratory work, laboratory reports	F- discussion, observation, correction of laboratory work; S - final exam; S- part-time exam

XRSA _07	TK_05, TK_06, TK_08, TK_09, TK_10	Lectures, laboratory work, laboratory reports	F- discussion, observation, correction of laboratory work; S - final exam
XRSA _08	TK_05, TK_06, TK_08, TK_09, TK_10	Lectures, laboratory work, laboratory reports	F- discussion, observation, correction of laboratory work; S - final exam; S- part-time exam
XRSA _09	TK_06, TK_07, TK_08, TK_09, TK_10	Lectures, laboratory work, laboratory reports	F- discussion, observation, correction of laboratory work; S - final exam
XRSA _10	TK_05, TK_08,	laboratory work,	F- discussion, observation, correction of laboratory work

** e.g. KHT_01 – module code as in Table in II.3 and II.4*
 # e.g. TK_01 – learning content symbol as in II.4
& Please include both formative (F) and summative (S) assessment

2. Student workload (ECTS credits)

Activity types	Mean number of hours* spent on each activity type
Contact hours with the teacher as specified in the programme	**45**
Preparation for laboratory	**30**
Completion of laboratory reports	**25**
Preparation for exam	**25**
Total hours	**125**
Total ECTS credits for the module	**5**

** Class hours – 1 hour means 45 minutes*
#Independent study – examples of activity types: (1) preparation for classes, (2) data analysis, (3) library-based work, (4)writing a class report, (5) exam preparation, etc.

3. Assessment criteria

Final grade will be assigned based on assessment of laboratory exercises and written examination. To pass the course at least 4 (out of 5) laboratory exercises must be completed.
To complete a laboratory exercise a pre-lab quiz must be passed and a satisfactory laboratory report from the experiment work must be handed in due time.

The final exam covers the lecture material and self-study assignments.

The labs contribute 0-5 points to the final grade
The exam contributes 0-25 points to the final grade
Final grades: **3.0** (16-20 pts); **3.5** (21-23 pts), **4.0** (24-26 pts), **4.5** (27-28 pts), **5.0** (29-30 pts)