

Detailed course description (SUBJECT CARD)

Course title: Characterization of chemical structures

Course code:

Classification of a course group:

Course type: field-related
obligatory

Field of study: Industrial and Engineering Chemistry

Level of study: second-cycle

Profile of study: general academic

Mode of study: full-time programme

Specialty (specialisation): all specialty

Year of study: first

Semester: **first**

Teaching modes and teaching hours:
lectures – 30 h;
laboratory – 45 h.

Language/s of instruction: English

Number of ECTS credits (according to the study programme): 5

1. Course objectives: To teach fundamentals of most important instrumental techniques destined to determination of structure of chemical compounds and properties of materials
2. Relation of the field-related learning outcomes to modes of teaching and methods of verification as well as to assessment of student's learning outcomes:

symbol	assumed learning outcomes <i>a student who completed the course:</i>	teaching modes	verification methods and learning outcomes assessment
Knowledge: a student knows and understands			
K2A_W08	Student knows modern methods of testing the structure and properties of materials, necessary to characterize raw materials and products of the chemical and related industries; knows the rules of organization of the chemical products market (REACH).	lecture	observation
Skills: a student can			
K2A_U03	Student is able to speak English fluently.	lecture, laboratory	observation, oral response
K2A_U01	Student has the ability to acquire and critically evaluate information from literature, databases and other sources and to form opinions and reports on this basis.	laboratory	observation, oral response
K2A_U06	Student has the ability to present research results in the form of a report, dissertation or presentation.	laboratory	observation, oral response
Social competences: a student is prepared to			
K2A_K06	Student is aware of the need for lifelong learning and professional development.	lecture, laboratory	observation, oral response

3. The content of study programme ensuring learning outcomes (*according to the study programme*):

Modern methods of structure analysis and property of materials determination necessary to characterization of feedstocks and products of chemical and other industries.

Analysis of spectroscopic data.

Acquiring and critical assessment of literature data, databases and other sources. Preparation of opinions and reports based on this procedure.

Analysis of NMR data, preparation of reports, dissertation or presentation.

Analysis of trends in structural studies.

4. Description of methods of determination of ECTS credits:

Type of activity	Number of hours / ECTS credits
Number of course hours regardless of a teaching mode	75/3

Student's work: preparation for a course	30/1
Student's work: interpretation of results	30/1
The other**	
Total hours:	135
Number of ECTS credits allocated to a course	5

Explanation:

* – student's workload - fill in the types of activities, e.g. *preparation for a course, interpretation of results, making a course report, preparation for an exam, studying sources, making a project, presentation and report, doing written assignment, etc.*

** – the other e.g. *extra course hours*

5. Summary indexes:

- number of course hours and ECTS credits at the course with a direct participation of academic teachers or other persons running the course and supervising students; 75/3
- number of course hours and ECTS credits at the course related to the scientific activity conducted at the Silesian University of Technology in a discipline or in disciplines to which a field of study is assigned - in the case of studies with a general academic profile; 75/3
- number of course hours and ECTS credits at the course developing practical skills- in the case of practical studies; 0
- number of course hours conducted by academic teachers employed by the Silesian University of Technology as their primary workplace. 75

6. Persons conducting particular modes of courses (name, surname, academic degree or degree in arts, title of professor, business e-mail address):

prof. dr hab. inż. Anna Chrobok, anna.chrobok@polsl.pl - wykład
dr hab. inż. Izabela Barszczewska-Rybarek, izabela.barszczewska-rybarek@polsl.pl - wykład
dr hab. inż. Nikodem Kuźnik, prof. Pol. Śl., nikodem.kuznik@polsl.pl - wykład, laboratorium
dr inż. Jakub Adamek, jakub.adamek@polsl.pl - wykład
dr inż. Agata Blacha-Grzechnik, agata.blacha-grzechnik@polsl.pl - wykład, laboratorium
dr inż. Anna Mielanzyk, anna.mielanzyk@polsl.pl - laboratorium

7. Detailed description of teaching modes:

1) lectures:

- detailed programme's content:

Backgrounds of nuclear magnetic resonance (NMR), scheme of spectrometer system, techniques ¹H and ¹³C NMR. Qualitative and quantitative analysis. Exemplary NMR spectra. ¹⁹F and ³¹P NMR spectra. NMR of polymers. Mass spectrometry (MS): scheme of apparatus, ionization techniques, ion fragmentation. Exemplary solving of MS spectra. Chromatography – theoretical background. Gaseous chromatography (GC), high performance liquid chromatography (HPLC, UPLC), thin layer chromatography (TLC). Apparatus construction, theoretical backgrounds, selection of analysis conditions. IR and UV-Vis spectroscopy. Theoretical backgrounds, examples of spectrum analysis. DSC/DMTA techniques in the study of polymeric materials, XPS, SERS, ellipsometry, contact angle measurements, STM, AFM, SEM, TEM - applications for the study of nanomaterials. X-ray diffraction on single crystals. Discussion of the phenomenon and application in the study of the structure of crystal bodies. Elements of quantitative and qualitative analysis of polycrystals.

- teaching methods, including distance learning:

The lecture is performed in the form of an interactive presentation.

- form and criteria for semester completion, including retake tests, as well as conditions for admission to the examination:

The material from the lecture is the basis for preparation for laboratory classes. Completing the material presented in the lectures is therefore done in the laboratory.

- course organisation and rules of participation in the course, with an indication whether a student's attendance is obligatory

Lectures are performed according to the schedule published during the first lecture and on the Remote Education Platform. In accordance with the study regulations, lectures are open and not obligatory.

2) laboratory:

- detailed programme's content:

Qualitative and quantitative ¹H NMR analysis. Interpretation of ¹H and ¹³C NMR spectra. Mass spectrometry (MS): sample preparation, analysis, interpretation of fragmentation spectra. GC, HPLC and UPLC chromatography. Discussion of the technique, sample preparation, chromatogram analysis. IR and UV-Vis spectroscopy. Sample preparation, analysis, interpretation of spectra. DSC / DMTA techniques in the study of polymeric materials. Examination of material surfaces using spectroscopic (XPS, SERS) and microscopic (STM) techniques - chemical composition and morphology analysis. Sample preparation, measurement, interpretation of obtained results. Structural x-ray analysis - sample preparation, stages of measurement, structure analysis.

- teaching methods, including distance learning:
Practical laboratory - getting acquainted with the technique by visiting the laboratory, preparing samples for analysis, taking measurements and analyzing the results obtained.
 - form and criteria for semester completion, including retake tests, as well as conditions for admission to the examination:
The semester completion is based on partial credits from laboratory classes. Positive grades from all laboratory classes are required to pass the course. There are three deadlines for passing laboratory classes.
 - course organisation and rules of participation in the course, with an indication whether a student's attendance is obligatory
Laboratory classes are conducted according to the schedule published during the first lecture and on the Remote Education Platform. In accordance with the study regulations, laboratory classes are compulsory.
8. Description of the method for determining the final grade (rules and criteria for evaluation, as well as the final grade calculation method in the case of a course comprising more than one teaching mode, taking into account all teaching modes and all exam dates and credit tests including retake exams and tests):
The final grade is the arithmetic average of the laboratory grades. Lectures are substantive preparation for laboratory classes, therefore this knowledge is verified at the stage of the laboratory test.
9. Method and procedure for making up for
- student's absence from the course,
Lectures are optional, so the student completes his knowledge based on literature. Laboratory classes are compulsory, so in the absence of the student contacts the teacher during the consultation period, where he agrees on an individual way to supplement the outstanding classes.
 - differences in study programmes for students changing their field of study, changing university or resuming studies at the Silesian University of Technology,
The student should meet the prerequisites and additional requirements so that he can take the classes.
10. Prerequisites and additional requirements, taking into account the course sequence:
The prerequisite is the completion of the basic course of physics, general and organic chemistry and polymer science at the academic level of the first degree.
A specific requirement for entering the laboratory is mastering the lecture material on the selected analytical technique.
11. Recommended sources and teaching aids:
1. R. S. Macomber, A complete introduction to modern NMR spectroscopy, New York : John Wiley & Sons, 1998
 2. R. M. Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce, Spectrometric Identification of Organic Compounds, New York : John Wiley & Sons
 3. B. Schrader, Infrared and Raman spectroscopy: methods and applications, Weinheim: VCH Verlagsgesellschaft, 1995.
 4. H. Gunther, NMR spectroscopy : basic principles, concepts, and applications in chemistry, Chichester : John Wiley & Sons, 1998.
 5. M. F. Ladd, R. A. Palmer, Structure determination by X-ray crystallography, New York : Plenum Press, 1994
 6. G. Schomburg, Gas chromatography : a practical course, Weinheim : VCH, 1990.
 7. Kromidas, HPLC made to measure : a practical handbook for optimization, Weinheim : Wiley-VCH, cop. 2006
12. Description of teachers' competences (e.g. publications, professional experience, certificates, trainings etc. related to the programme contents implemented as a part of the course):
The lecturers are specialists in the field of spectroscopic techniques that they discuss. Their competences are confirmed by diplomas and doctoral degrees in chemical sciences, which result from research work carried out using spectroscopic techniques. Additional confirmation of competences are numerous, reviewed scientific publications conducting research using spectroscopic techniques.
13. Other information:
none