A COURSE SYLLABUS – DOCTORAL SCHOOL
regarding the qualification cycle from 2022/2023 to 2025/2026
and
regarding the qualification cycle from 2024/2025 to 2027/2028

GENERAL INFORMATION ABOUT COURSE	
Course title	***OPTIONAL SPECIALIZED SUBJECT:*** ***Spectroscopy of polyatomic molecules***
Name of the unit running the course	Doctoral School at University of Rzeszów
Type of course *(obligatory, optional)*	obligatory - optional specialist subject
Year and semester of studies	year I: semester II and year III: semester VI
Discipline	Physical sciences
Language of Course	Polish language
Name of Course coordinator	dr hab. Rafał Hakalla, prof. UR
Name of Course lecturer	dr hab. Rafał Hakalla, prof. UR
Prerequisites	Knowledge of physics, quantum physics and molecular spectroscopy at the level of a second degree course in physics or chemistry.

BRIEF DESCRIPTION OF COURSE
(100-200 words)

The course is devoted to advanced issues in the spectroscopy of polyatomic molecules, with particular emphasis on methods allowing the study of their structure and dynamics. It covers both theoretical and practical aspects, including interpretation of spectra, application of group theory in symmetry analysis, as well as modern spectroscopic techniques. The course provides an understanding of quantum phenomena occurring in polyatomic molecules and how they relate to experimental results.

COURSE LEARNING OUTCOMES AND METHODS OF EVALUATING LEARNING OUTCOMES

Learning outcome	The description of the learning outcome defined for the course	Relation to the degree programme outcomes (symbol)	Learning Format (Lectures, classes,...)	Method of assessment of learning outcomes (e.g. test, oral exam, written exam, project,...)
Knowledge (no.)	knows and understands, has knowledge			
1	Issues of spectroscopy of polyatomic molecules to the extent of revising existing paradigms, both theoretical and experimental.	**P8S_WG/1**	Conversation	project
2	The main developmental trends of contemporary spectroscopy of polyatomic molecules.	**P8S_WG/2**	Conversation	project
3	Has interdisciplinary knowledge, knows and understands the terminology used in the discipline of physical sciences in the native and foreign language, especially in issues related to the spectroscopy of polyatomic molecules.	**P8S_WG/3**	Conversation	project
4	Knows and understands the impact of developments in technology and engineering on	**P8S_WK/1**	Conversation	project

	the progress of civilisation, including the discovery of new issues in polyatomic particle spectroscopy.			
Skills (no.)	can			
1	Use knowledge from various fields of science to creatively identify and innovatively solve complex problems or perform tasks of a research nature in the field of spectroscopy of polyatomic molecules, and in particular: (**I**) define the purpose and object of scientific research; (**II**) formulate a research hypothesis; (**III**) develop methods, techniques research tools and apply them creatively; (IV) make inferences on the basis of scientific research.	**P8S_UW/1**	Conversation	project
2	Is able to select and use the available professional literature on the spectroscopy of polyatomic molecules to diagnose and solve research problems and innovative actions related to his/her scientific activity, and to apply the appropriate course of action to create new elements of scientific output.	**P8S_UW/2**	Conversation	project
3	Critically analyse and evaluate the results of spectroscopic research, expert activities and other creative work and their contribution to the advancement of knowledge.	**P8S_UW/3**	Conversation	project
4	Be able to use English at B2 level of the European Language Learning System to a degree that enables them to participate in the international scientific community related to the spectroscopy of polyatomic molecules.	**P8S_UK/6**	Conversation	project
Social competence (no.)	is ready to			
1	Recognising the importance of knowledge in solving cognitive and practical problems using molecular spectroscopy issues as an example.	**P8S_KK/3**	Conversation	project

LEARNING FORMAT – NUMBER OF HOURS						
Semester (no.)	Lectures	Seminars	Lab classes	Internships	others	ECTS
II and VI	-	-	15	-	-	2

METHODS OF INSTRUCTION

- PRESENTATION;
- DISCUSSION;
- SOLVING COMPUTATIONAL TASKS;
- PROBLEM SOLVING;

COURSE CONTENT

A. Lecture problems (5 hours)

Contents:

1. Introduction to the spectroscopy of polyatomic molecules.
2. Molecular symmetry and its influence on spectroscopic spectra.
3. Vibrational spectroscopy: normal vibrations, transition intensities, selection rules.
4. Rotational spectroscopy of polyatomic molecules: structure and analysis of spectra.
5. Internal dynamics of polyatomic molecules and coupling between vibrations and rotations.

B. Problems of auditory exercises (10 hours)

Content:

Solving given problems by means of modern computational methods of spectroscopy of polyatomic molecules. Tasks will be selected according to the lecture topics.

1. Symmetry analysis of molecules and the use of group theory in spectroscopy.
2. Solving problems in vibrational spectroscopy.
3. Interpretation of rotational and vibrational-rotational spectra using available computational tools.
4. Modelling of spectra of polyatomic molecules taking into account coupling between vibrational and rotational motion.

COURSE ASSESSMENT CRITERIA

The subject ends with an examination after each semester of implementation (semester 2, semester IV, semester VI, semester VII). Possible semester grades are: 2.0, 3.0, 3.5, 4.0, 4.5, 5.0.

The final grade for the exercises will be given on the basis of partial grades:

- very good: the doctoral student has mastered more than 90% of the range of knowledge; knows how to solve calculus tasks;
- **good plus**: the student has mastered more than 80% of the range of knowledge; he/she is able to solve calculation tasks;
- **good**: the student has mastered more than 80% of the scope of knowledge and is able to solve typical calculation tasks;
- **sufficient plus**: a doctoral student has mastered more than 70% of the scope of knowledge and is able to solve typical calculation tasks;
- **sufficient:** a student knows the basic concepts of the subject and is able to solve simple calculation tasks;
- **unsatisfactory**: the student knows the basic concepts of the subject and cannot solve simple calculation tasks;

TOTAL PhD STUDENT WORKLOAD REQUIRED TO ACHIEVE THE INTENDED LEARNING OUTCOMES – NUMBER OF HOURS AND ECTS CREDITS

Activity	Number of hours
Scheduled course contact hours	15
Other contact hours involving the teacher (consultation hours, examinations)	5

Non-contact hours – student`s own work (preparation for classes or examinations, project, etc.)	40
Total number of hours	**60**
Total number of ECTS credits*	**2**

INSTRUCTIONAL MATERIALS	
Compulsory literature:	1. Atkins, P., de Paula, J., & Keeler, J. (2022). *Atkins' Physical Chemistry* (12th ed.). Oxford: Oxford University Press. 2. G. Gauglitz, D. S. Moore, *Handbook of Spectroscopy*, Wiley-VCH Verlag GmBH, 2014. 3. J. Sadlej, *Spektroskopia molekularna*, WNT, 2002. 4. W. Kołos, J. Sadlej, *Atom i cząsteczka*, WNT, 1998. 5. G. Herzberg, *Molecular Spectra and Molecular Structure, vol. I: Spectra of Diatomic Molecules*, (2nd edition), Krieger Publishing Company, Malabar, Florida, 1989. 6. Haken, H., Wolf, H.C., & Brewer, W.D. (2005). *The Physics of Atoms and Quanta: Introduction to Experiments and Theory* (7th ed.). Berlin, Heidelberg: Springer. 7. Haken, H., & Wolf, H.C. (2004). *Molecular Physics and Elements of Quantum Chemistry: Introduction to Experiments and Theory* (2nd ed., trans. W.D. Brewer). Berlin, Heidelberg: Springer. 8. Z. Leś, *Podstawy fizyki atomu. Wprowadzenie do współczesnej spektroskopii atomowej,* PWN, 2015.
Complementary literature:	1. P. Kowalczyk, *Fizyka cząsteczek. Energie i widma*, PWN, 2000. 2. W. Demtröder, *Atoms, Molecules and Photons An Introduction to Atomic-, Molecular- and Quantum Physics*, Springer Verlag, 2010.

*(1 ECTS CREDIT CORRESPONDS TO 25 - 30 HOURS OF THE TOTAL WORKLOAD OF A DOCTORAL STUDENT, NEEDED TO ACHIEVE THE ESTABLISHED EFFECTS).

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Date and signature of the Course lecturer

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Approved by the Head of the Department or an authorised person