

**A COURSE SYLLABUS – DOCTORAL SCHOOL**  
REGARDING THE QUALIFICATION CYCLE FROM 2025/2026 TO 2028/2029

<b>GENERAL INFORMATION ABOUT COURSE</b>				
Course title	<b>DOCTORAL SEMINAR</b>			
Name of the unit running the course	Rzeszów University Doctoral School			
Type of course ( <i>obligatory, optional</i> )	Compulsory subject			
Year and semester of studies	Years I – IV, semesters: I–VII			
Discipline	<b>Physical sciences</b>			
Language of Course	Polish language/English language			
Name of Course coordinator	Dr Rafał Hakalla, Professor at the University of Rzeszów			
Name of Course instructor	Dr Rafał Hakalla, Professor at the University of Rzeszów			
Prerequisites	Academic education at the master's degree level in physics. Knowledge, skills and social competences at level 7 of the Polish Qualifications Framework. Knowledge of a foreign language at level B2, enabling the use of foreign-language sources of scientific information, preparation of publications and presentation of scientific achievements at specialist conferences.			
<b>BRIEF DESCRIPTION OF COURSE</b> (100-200 words)				
<p>The aim of the doctoral seminar is to deepen theoretical, experimental and methodological knowledge in the field of high-resolution molecular spectroscopy and to present and critically analyse current scientific research results. The course covers modern experimental and computational techniques used in rotational, vibrational and electronic spectroscopy, with particular emphasis on conducting experimental research, such as recording spectra using advanced measuring equipment, optimising experimental conditions and assessing measurement uncertainties. An important element of the doctoral seminar is the discussion of international literature and the presentation of the progress of doctoral students' own research, with particular emphasis on research problems, interpretation of results and their significance for physical sciences and related sciences (astrophysics, physical chemistry, atmospheric physics). The aim of the course is to develop the skills of independent scientific research, critical thinking and communication of results in the form of oral presentations and scientific discussions. The doctoral seminar prepares doctoral students for active participation in the scientific community and for the completion of a doctoral dissertation at an international level.</p>				
<b>COURSE LEARNING OUTCOMES AND METHODS OF EVALUATING LEARNING OUTCOMES</b>				
Learning outcome	The description of the learning outcome defined for the course	Reference to learning outcomes for qualifications at Level 8 of the Polish Qualification Framework (PRK) (symbol)	Learning Format (Lectures, classes,...)	Method of assessment of learning outcomes (e.g. test, oral exam, written exam, project,...)
<b>Knowledge:</b> (no.)	<i>knows and understands</i>			

P8S_WG1	Possesses extensive theoretical knowledge, supported by research experience, and is familiar with current scientific achievements, including global ones, in the field of education in the scientific discipline of physical sciences, with particular emphasis on high-resolution molecular spectroscopy, to a degree that allows for the confirmation or refutation of existing paradigms.	P8S_WG	seminar	oral presentation, discussion
P8S_WG2	He/she is familiar with the directions of scientific research in the scientific discipline of physical sciences, with particular emphasis on high-resolution molecular spectroscopy and the latest discoveries, including global ones, in the discipline in which the education takes place.	P8S_WG	seminar	oral presentation, discussion
P8S_WG3	Knows, understands and is able to apply concepts used by scientists and specialists in the discipline of physical sciences and related disciplines, with particular emphasis on high-resolution molecular spectroscopy in their native and foreign languages, which are leading in the discipline.	P8S_WG	seminar	oral presentation, discussion
<b>Skills: (no.)</b>	<b><i>is able to</i></b>			
P8S_UW1	Based on their knowledge in various fields of science, they are able to identify and solve scientific research problems in the field of high-resolution molecular spectroscopy, define the objective, formulate a hypothesis and the subject of scientific research, select and refine research techniques, methods and tools, and draw conclusions based on the results of scientific research.	P8S_UW	seminar	oral presentation, discussion, written assignments
P8S_UW2	They are able to select and use available scientific literature to diagnose and solve research problems and innovative activities in their research work in the field of high-resolution molecular spectroscopy, as well as apply the appropriate tools to create new elements of scientific output.	P8S_UW	seminar	oral presentation, discussion, written assignments
P8S_UW3	Using their interdisciplinary knowledge to analyse and evaluate the results of scientific research in the field of high-resolution molecular spectroscopy, expert reports and other scientific studies, they are able to formulate opinions, including critical judgements.	P8S_UW	seminar	oral presentation, discussion, written assignments

<b>P8S_UK6</b>	They are able to speak in public to present the results of scientific research in the field of high-resolution molecular spectroscopy and participate in discussions on scientific, social and professional topics in an international environment, using a foreign language at level B2 of the Common European Framework of Reference for Languages.			<b>P8S_UK</b>	seminar	oral presentation, discussion, written assignments
<b>Social competence: (no.)</b>	<i>is ready to</i>					
<b>P8S_KK1</b>	Is prepared to critically evaluate achievements in the scientific discipline of physics and to critically evaluate the contribution of their own research results in the field of high-resolution molecular spectroscopy to the scientific development of the discipline in which they are studying.			<b>P8S_KK</b>	seminar	oral presentation, discussion, written assignments
<b>P8S_KK3</b>	Thanks to their extensive knowledge, they solve various cognitive and practical problems in the field of high-resolution molecular spectroscopy.			<b>P8S_KK</b>	seminar	oral presentation, discussion, written assignments
<b>LEARNING FORMAT – NUMBER OF HOURS</b>						
Semester (no.)	Lectures	Seminars	Lab classes	Placements	other	ECTS
I - VII	-	-	-	-	7 x 15 godz. -105 godz.	7 x 2 ECTS – 14 ECTS
<b>METHODS OF INSTRUCTION</b>						
<ul style="list-style-type: none"> <li>- <i>ACADEMIC DISCUSSION,</i></li> <li>- <i>STUDY OF SOURCES AND ACADEMIC LITERATURE,</i></li> <li>- <i>MULTIMEDIA PRESENTATION,</i></li> <li>- <i>PREPARATION AND PRESENTATION OF RESEARCH OBJECTIVES, RESEARCH METHODS, RESEARCH RESULTS,</i></li> <li>- <i>PARTIAL STUDIES,</i></li> <li>- <i>PROGRESS IN THE PREPARATION OF A DOCTORAL THESIS</i></li> </ul>						
<b>COURSE CONTENT</b>						
<p>The doctoral seminar will cover content aimed at developing the knowledge, skills and research competences of doctoral students in the field of high-resolution molecular spectroscopy and providing support in the preparation of doctoral theses. At each stage of education, the following knowledge, skills and social competences will be developed:</p> <ol style="list-style-type: none"> <li>1. Principles of high-resolution molecular spectroscopy (theoretical foundations, fundamental principles, laws and rules; applications in atmospheric research, astrophysics and quantum molecular chemistry).</li> <li>2. Advanced methods of high-resolution spectroscopy (Fourier-transform spectroscopy techniques; laser techniques; absorption and emission spectroscopy).</li> <li>3. Advanced methods of spectroscopic data analysis (frequency calibration; determination of measurement uncertainties; numerical methods in spectrum analysis; identification and analysis of perturbations).</li> </ol>						

4. Practical applications of molecular spectroscopy (basics of studying intramolecular interactions, determining molecular constants and perturbation parameters and their significance in theoretical models; use of spectroscopy to determine molecular parameters in laboratory conditions).
5. Modern trends in spectroscopy (femtosecond and sub-Doppler spectroscopy; molecular spectroscopy in optical traps and magnetic fields; the use of spectroscopy in time and frequency metrology).
6. Presentation of research results (preparation of scientific reports and publications; oral presentation of research results at seminars and conferences; practical tips on reviewing and improving scientific texts).
7. Protection of intellectual property and commercialisation of research results (principles of copyright and patent protection in physical sciences; possibilities for commercialisation of spectroscopic research results).

Topics covered in classes, divided into semesters:

#### **Semester I**

Topic 1: Introduction to high-resolution emission Fourier-transform spectroscopy of diatomic molecules.

Topic 2: Energy structure of a selected diatomic molecule: configurations and electronic states, vibrational and rotational levels.

Topic 3: Review of literature on the recording and analysis of spectra of a selected molecule.

#### **Semester II**

Topic 1: Principle of operation of a Fourier-transform spectrometer, configuration and optimisation of experimental parameters.

Topic 2: Development of an individual experimental methodology for obtaining the emission spectrum of a selected diatomic molecule.

Topic 3: Construction of a proprietary emission spectrum source for a selected diatomic molecule.

#### **Semester III**

Topic 1: Excitation and recording of emission spectra of a selected diatomic molecule, optimisation of experimental conditions.

Topic 2: Calibration of the frequency axis of recorded emission spectra of a selected diatomic molecule.

Topic 3: Preliminary identification and interpretation of the obtained spectra: analysis of electronic transitions and the structure of spectral bands and branches.

#### **Semester IV**

Topic 1: Identification and measurement of spectra: determination of the wavenumbers of ro-vibronic transitions associated with the first vibrational level of the excited electronic state.

Topic 2: Determination of molecular parameters for the first vibrational level of the excited electronic state and the ground state, assessment of uncertainty and quality of experimental data fitting.

Topic 3: Comparison of experimental results with literature data and theoretical calculations, writing a scientific article presenting the obtained results.

#### **Semester V**

Topic 1: Identification and measurement of spectra: determination of wavenumbers of ro-vibronic transitions associated with the second vibrational level of the excited electronic state.

Topic 2: Determination of molecular parameters for the second vibrational level of the excited electronic state and the ground state, assessment of uncertainty and quality of experimental data fitting.

Topic 3: Comparison of experimental results with literature data and theoretical calculations, writing a scientific article presenting the obtained results.

#### **Semester VI**

Topic 1: Identification and measurement of spectra: determination of wavenumbers of ro-vibronic transitions associated with the third vibrational level of the excited electronic state.

Topic 2: Determination of molecular parameters for the third vibrational level of the excited electronic state and the ground state, assessment of uncertainty and quality of experimental data fitting.

Topic 3: Comparison of experimental results with literature data and theoretical calculations, writing a scientific article presenting the obtained results.

### Semester VII

Topic 1: Determination of experimental terms/energy levels based on the obtained experimental data, writing a scientific article presenting the obtained results.

Topic 2: Writing a doctoral dissertation.

### COURSE ASSESSMENT CRITERIA

The assessment covers the doctoral student's continuous work in each semester and academic year in the following areas: conducting research, expanding knowledge, studying literature, commitment and progress in preparing the doctoral dissertation.

The course ends after each semester of implementation:

**pass – pass,**

**fail – fail.**

The following percentage of points obtained is used to assess the course:

- up to 60% - fail - the doctoral student is not making progress in scientific research, is not expanding their knowledge, is not studying the literature, is not participating in substantive discussions, is not fulfilling their scientific obligations;

- 61% - 100% - pass - the doctoral student is making progress in scientific research, expanding their knowledge, studying basic and supplementary literature, participating in substantive discussions, fulfilling all scientific duties

### TOTAL DOCTORAL STUDENT WORKLOAD REQUIRED TO ACHIEVE THE EXPECTED LEARNING OUTCOMES – NUMBER OF HOURS AND ECTS CREDITS

Activity	Number of hours
Scheduled course contact hours	7 x 15 hrs. – 105 hrs.
Other contact hours involving the instructor (duty hours, examinations)	6 hrs.
Non-contact hours – student's own work (preparation for classes or examinations, project, etc.)	309 hrs.
<b>Total number of hours</b>	<b>420 hrs.</b>
<b>Total number of ECTS credits</b>	<b>7 x 2 ECTS – 14 ECTS</b>

### INSTRUCTIONAL MATERIALS

Compulsory literature:	<ol style="list-style-type: none"> <li>1. P. F. Bernath, <i>Spectra of Atoms and Molecules</i>, 4th Edition, Oxford University Press, 2020.</li> <li>2. G. Herzberg, <i>Molecular Spectra and Molecular Structure, vol. I: Spectra of Diatomic Molecules</i>, (2<sup>nd</sup> edition), Krieger Publishing Company, Malabar, Florida, 1989.</li> <li>3. J. Tennyson, <i>Astronomical Spectroscopy: An Introduction To The Atomic And Molecular Physics Of Astronomical Spectroscopy</i>, World Scientific Europe Ltd, 2019.</li> <li>4. H. Lefebvre-Brion, R.W. Field, <i>The Spectra and Dynamics of Diatomic Molecules</i>, Elsevier, 2004.</li> <li>5. P. Kowalczyk „Fizyka cząsteczek. Energie i widma”, PWN, 1999.</li> <li>6. P. W. Atkins, <i>Physical Chemistry</i>, 11th edition, Oxford University Press, 2018.</li> </ol>
------------------------	--

	<ol style="list-style-type: none"> <li>7. <i>Handbook of High-Resolution Spectroscopy</i>, Vol. 1-3, ed. by M. Quack and F. Merkt, Wiley, 2011.</li> <li>8. J. T. Hougen, <i>The Calculation of Rotational Energy Levels and Rotational Line Intensities in Diatomic Molecules</i>, National Institute of Standards and Technology (NIST), Monograph 115, 1970.</li> <li>9. J. M. Brown and A. Carrington, <i>Rotational Spectroscopy of Diatomic Molecules</i>, Cambridge University Press, 2003.</li> <li>10. N. Colin, N. Banwell and E. M. McCash, <i>Fundamentals of Molecular Spectroscopy</i>, 4th Edition, McGraw-Hill, 2021.</li> <li>11. H. Haken and H. C. Wolf, <i>Molecular Physics and Elements of Quantum Chemistry: Introduction to Experiments and Theory</i>, 2nd Edition, Springer, 2004.</li> </ol>
Complementary literature:	<ol style="list-style-type: none"> <li>1. J. Sadlej „Spektroskopia molekularna”, WNT, 2002</li> <li>2. W. Kołos, J. Sadlej „Atom i cząsteczka”, WNT, 1998</li> <li>3. W. Kołos „Chemia kwantowa”, PWN, 1978.</li> <li>4. A. Gołębiewski „Elementy mechaniki i chemii kwantowej”, PWN, 1982.</li> <li>5. Z. Leś „Wstęp do spektroskopii atomowej”, PWN 2014.</li> <li>6. H. Haken and H. C. Wolf, <i>The Physics of Atoms and Quanta</i>, 7th Edition, Springer, 2005.</li> </ol>

**\*(1 ECTS POINT CORRESPONDS TO 25–30 HOURS OF TOTAL WORK BY THE DOCTORAL STUDENT REQUIRED TO ACHIEVE THE INTENDED RESULTS)**

.....  
Date and signature of the Course instructor

.....  
Approved by the Head of the Department or an authorised person