A COURSE SYLLABUS – DOCTORAL SCHOOL

REGARDING THE QUALIFICATION CYCLE FROM 2024/2025 TO 2028/2029

GENERAL INFORMATION ABOUT COURSE	
Course title	**DOCTORAL SEMINAR**
Name of the unit running the course	Doctoral School at University of Rzeszów
Type of course *(obligatory, optional)*	obligatory subject
Year and semester of studies	year I -IV, semester: I - VII
Discipline	Physical science
Language of Course	Polish/English language
Name of Course coordinator	Dr. Rafał Hakalla, prof. UR
Name of Course lecturer	Dr. Rafał Hakalla, prof. UR
Prerequisites	The scope of knowledge resulting from the curriculum of the master's degree in physics. Knowledge of the English language at a level that allows the use of foreign-language sources of scientific information, preparation of publications and presentation of scientific achievements at specialized conferences.

BRIEF DESCRIPTION OF COURSE
(100-200 words)

Development of knowledge, skills and research competence of doctoral students in the field of high-resolution molecular spectroscopy and support in the preparation of a PhD dissertation.

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			
P8S_WG1	To the extent that it is possible to revise existing paradigms - a worldwide body of work, including theoretical foundations and general issues and selected specific issues - specific to high-resolution molecular spectroscopy;	**P8S_WG**	seminar	oral statement, discussion
P8S_WG2	knows the subject of the main development trends of high-resolution spectroscopy;	**P8S_WG**	seminar	oral statement, discussion
P8S_WG3	knows, understands and can apply professional terms used in high resolution molecular spectroscopy, in native and foreign languages;	**P8S_WG**	seminar	oral statement,
Skills (no.)	can			
P8S_UW1	based on his knowledge of various fields of science, is able to identify and solve problems of high-resolution molecular spectroscopy, define the purpose, formulate the	**P8S_UW**	seminar	oral statement, discussion

	hypothesis and the object of scientific research, improve spectroscopic research techniques, methods and tools, and make conclusions based on the results of scientific research;			
P8S_UW2	select and use scientific literature to diagnose and solve research problems and innovative activities in their research work, and apply the appropriate workshop to create new elements of scientific achievements;	**P8S_UW**	seminar	oral statement, discussion
P8S_UW3	critically analyze and evaluate the results of scientific research, expert activities and other works of a creative nature and their contribution to the development of high-resolution spectroscopy;	**P8S_UW**	seminar	oral statement, discussion
P8S_UK6	communicate on the topics of molecular spectroscopy to a degree that enables active participation in the international scientific community , to present the results of scientific research and participate in the discussion of scientific and professional topics in an international environment, using a foreign language at the B2 level of the European Language Education System;	**P8S_UK**	seminar	oral statement, discussion
Social competence (no.)	is ready to			
P8S_KK1	to critically evaluate the achievements within the framework of high-resolution molecular spectroscopy and to critically evaluate the contribution of the results of his own research activities to the development of this discipline;	**P8S_KK**	seminar	oral statement, discussion
P8S_KK3	solves cognitive and practical problems with his knowledge;	**P8S_KK**	seminar	oral statement, discussion

LEARNING FORMAT – NUMBER OF HOURS

Semester (no.)	Lectures	Seminars	Lab classes	Internships	others	ECTS
I - VII	-	-	-	-	**7 x 15 hrs - 105 hrs.**	14

METHODS OF INSTRUCTION

- SCIENTIFIC DISCUSSION**,**
- STUDY OF SCIENTIFIC LITERATURE**,**
- MULTIMEDIA PRESENTATION**,**

- PREPARATION AND PRESENTATION OF THE PURPOSE OF RESEARCH , RESEARCH METHODS, RESEARCH RESULTS,
- PROGRESS IN THE PREPARATION OF THE DISSERTATION.

COURSE CONTENT

Doctoral seminar

The aim of the course is to develop the knowledge, skills and research competence of doctoral students in the field of high-resolution molecular spectroscopy and support in the preparation of the doctoral dissertation, so at each stage of training the following will be developed:

1. Introduction to high resolution molecular spectroscopy
   (Fundamental principles and research objectives; Application to atmospheric research, astrophysics and quantum molecular chemistry).

2. Advanced methods of high-resolution spectroscopy (Fourier-transform spectrometry techniques; laser techniques: absorption and emission spectroscopy).

3. Advanced analysis of spectroscopic data (frequency calibration; determination of measurement uncertainties; numerical methods in spectral analysis; deperturbation analysis).

4. Practical applications of molecular spectroscopy (fundamentals of the study of intramolecular interactions, determination of molecular constants and perturbation parameters and their significance in theoretical models; use of spectroscopy to determine molecular parameters under laboratory conditions).

5. Modern directions in spectroscopy (femtosecond and sub-Doppler spectroscopy; molecular spectroscopy in optical traps and magnetic fields; application 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 for reviewing and improving scientific texts).

7. Intellectual property protection and commercialization of research results (principles of copyright and patent protection in the physical sciences; opportunities for commercialization of spectroscopic research results).

Contents 1-7 will be implemented during the following specific topics:

Semester I

Topic: Development of an individual methodology for the measurement and spectroscopic analysis of a selected molecule taking into account the relevant research techniques.

Topic : Designing and commissioning a source of spectra of a selected diatomic molecule.

Topic : Obtaining the ro-vibronic spectrum of a molecule in the selected measurement range.

Semester II

Topic: Identifying the spectrum associated with the first vibrational level of a key electronic state.

Topic: Selection of theoretical analytical methods appropriate for high resolution spectroscopy.

Semester III

Topic : Performing deperturbation analysis for the first vibrational level of the key electronic state.

Topic : Obtaining and presenting the results and making conclusions and predictions.

Topic : Writing a scientific article presenting the obtained results for the first level of the vibrational level.

Semester IV

Topic: Identifying the spectrum associated with the next vibrational level of the key electronic state.

Topic: Performing deperturbation analysis for the next vibrational level of the key electronic state.

Topic: Obtaining and presenting results and making conclusions and predictions.

Topic: Writing a scientific article presenting the obtained results.

Semester V

Topic: Conducting deperturbation analysis for the next two vibrational levels of the key electronic state.

Topic: Obtaining and presenting the results and making conclusions and predictions.

Topic: Writing two scientific papers presenting the obtained results.

Semester VI

Topic: Conducting a global deperturbation analysis involving all analyzed vibrational levels of the key electronic state.

Topic: Writing a scientific article presenting the obtained results.

Semester VII and VIII

Topic: Writing a PhD dissertation.

COURSE ASSESSMENT CRITERIA

The evaluation is based on the continuous work of the doctoral student in each semester and academic year in terms of: implementation of research, expansion of knowledge, study of literature, involvement and progress in the preparation of the dissertation. Possible semester grades are: 2.0, 3.0, 3.5, 4.0, 4.5, 5.0.
Sample percentage requirements for the grading scale:
To obtain a passing grade, a conversion factor is used for the corresponding percentage of points obtained:
- up to 50% - insufficient, (the doctoral student does not make progress in scientific research, does not expand his knowledge, does not study the readings, does not participate in substantive discussion, does not fulfill his scientific duties);
- 51% - 60% - sufficient, (the doctoral student makes negligible progress in scientific research, expands knowledge, studies primary literature, the discussion held is limited to a narrow range of substantive knowledge, fulfills basic scientific duties);
- 61% - 70% - sufficient plus, (the doctoral student makes progress in scientific research, expands knowledge, studies basic literature, substantively participates in the discussion , fulfills scientific duties);
- 71% - 80% - good, (doctoral student makes significant progress in scientific research, expands knowledge, studies primary and secondary literature, substantively participates in discussion, fulfills all scientific duties);
- 81% - 90% - good plus, (the doctoral student makes significant progress in scientific research, systematically expands knowledge, studies basic and complementary literature, substantively participates in discussion, fulfills all scientific duties);
- 91% - 100% - very good (the doctoral student makes significant progress in scientific research, systematically expands knowledge, studies basic, complementary and beyond the obligatory literature, substantively participates in discussion, fulfills all scientific duties);

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	**7 x 15 hrs - 105 hrs.**
Other contact hours involving the teacher (consultation hours, examinations)	**6**
Non-contact hours – student`s own work (preparation for classes or examinations, project, etc.)	**309**
Total number of hours	**420**
Total number of ECTS credits	**14**

INSTRUCTIONAL MATERIALS

Compulsory literature:	1. P. W. Atkins, *Physical Chemistry*, 11th edition, Oxford University Press, 2018. 2. *Handbook of High-Resolution Spectroscopy*, Vol. 1-3, ed. by M. Quack and F. Merkt, Wiley, 2011. 3. P. F. Bernath, *Spectra of Atoms and Molecules*, 4th Edition, Oxford University Press, 2020. 4. G. Herzberg, *Molecular Spectra and Molecular Structure, vol. I: Spectra of Diatomic Molecules*, (2nd edition), Krieger Publishing Company, Malabar, Florida, 1989. 5. J. T. Hougen, *The Calculation of Rotational Energy Levels and Rotational Line Intensities in Diatomic Molecules*, National Institute of Standards and Technology (NIST), Monograph 115,

	1970. 6. H. Lefebvre-Brion, R.W. Field, *The Spectra and Dynamics of Diatomic Molecules*, Elsevier, 2004. 7. J. M. Brown and A. Carrington, *Rotational Spectroscopy of Diatomic Molecules*, Cambridge University Press, 2003. 8. N. Colin, N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Edition, McGraw-Hill, 2021. 9. H. Haken and H. C. Wolf, *Molecular Physics and Elements of Quantum Chemistry: Introduction to Experiments and Theory,* 2nd Edition, Springer, 2004. 10. H. Haken and H. C. Wolf, *The Physics of Atoms and Quanta*, 7th Edition, Springer, 2005.
Complementary literature:	1. J. Sadlej „Spektroskopia molekularna", WNT, 2002 2. W. Kołos, J. Sadlej „Atom i cząsteczka", WNT, 1998 3. W. Kołos „Chemia kwantowa", PWN, 1978 4. P. Kowalczyk „Fizyka cząsteczek. Energie i widma", PWN, 1999. 5. A. Gołębiewski „Elementy mechaniki i chemii kwantowej", PWN, 1982. 6. Z. Leś „Wstęp do spektroskopii atomowej", PWN 2014.

*(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