

## ETY507 - Group Theory and Applications for Materials Characterization

### COURSE OUTLINE

#### (1) GENERAL

<b>SCHOOL</b>	SCHOOL OF ENGINEERING		
<b>ACADEMIC UNIT</b>	DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING		
<b>LEVEL OF STUDIES</b>	UNDERGRADUATE		
<b>COURSE CODE</b>	ETY507	<b>SEMESTER</b>	7
<b>COURSE TITLE</b>	Group Theory and Applications for Materials Characterization		
<b>INDEPENDENT TEACHING ACTIVITIES</b> <i>if credits are awarded for separate components of the course, e.g. lectures, laboratory exercises, etc. If the credits are awarded for the whole of the course, give the weekly teaching hours and the total credits</i>		<b>WEEKLY TEACHING HOURS</b>	<b>CREDITS</b>
Lectures		3	3
<i>Add rows if necessary. The organization of teaching and the teaching methods used are described in detail at (d).</i>			
<b>COURSE TYPE</b> <i>general background, special background, specialized general knowledge, skills development</i>	specialized general knowledge		
<b>PREREQUISITE COURSES:</b>	-		
<b>LANGUAGE OF INSTRUCTION and EXAMINATIONS:</b>	GREEK		
<b>IS THE COURSE OFFERED TO ERASMUS STUDENTS</b>	-		
<b>COURSE WEBSITE (URL)</b>			

#### (2) LEARNING OUTCOMES

##### Learning outcomes

*The course learning outcomes, specific knowledge, skills and competences of an appropriate level, which the students will acquire with the successful completion of the course are described.*

*Consult Appendix A*

- *Description of the level of learning outcomes for each qualifications cycle, according to the Qualifications Framework of the European Higher Education Area*
- *Descriptors for Levels 6, 7 & 8 of the European Qualifications Framework for Lifelong Learning and Appendix B*
- *Guidelines for writing Learning Outcomes*

Knowledge of molecular symmetry allows the student to quantify and accurately describe the structure of the molecules. In other words, molecular symmetry is the basis for a general way of classifying different molecules into groups, respectively with their stereochemical structure. In addition, knowledge of molecular symmetry gives ability to understand many phenomena and simplify the study many problems of chemistry, directly related to shapes and arrangements in the orbital space of atoms and molecules. So some of these problems are:

- The study of how AO (individual orbitals) interact for formation of molecular orbital MO (chemical bond).
- The interpretation of vibration or oscillation spectra (IR and Raman spectra).
- The selection rules governing electronic transfers to individuals and molecules (electronic spectra).

Understanding molecular symmetry problems based on group theory will be a prerequisite for further research and interpretation of the complex exercises of materials science. The ability to determine active vibrations in the IR and Raman spectra in the light of molecular symmetry gives the student the confidence he or she needs and the experience of analyzing the peaks and interpreting vibration spectra. It acquires another sense of molecular spectroscopy which continues to be a powerful material characterization technique. In this direction, the teaching of the course moves, which in combination with the work of applying all that the applied theory of groups negotiates, gives the student the modern thinking that the problems of characterization of the materials require.

Upon successful completion of the course the student will be able to:

Distinguish, to interpret, evaluate and conclude the value and importance of the above knowledge from the teaching of the molecular symmetry course in combination with the spectroscopy in his undergraduate laboratory course but also in his professional career as a Materials Engineer and with regard to Application, The student must be able to use this knowledge beyond the narrow confines of this course, and specifically in the context of the challenges he will face in practicing the profession of Engineering, Materials, industry or research.

#### General Competences

*Taking into consideration the general competences that the degree-holder must acquire (as these appear in the Diploma Supplement and appear below), at which of the following does the course aim?*

<i>Search for, analysis and synthesis of data and information, with the use of the necessary technology</i>	<i>Project planning and management</i>
<i>Adapting to new situations</i>	<i>Respect for difference and multiculturalism</i>
<i>Decision-making</i>	<i>Respect for the natural environment</i>
<i>Working independently</i>	<i>Showing social, professional and ethical responsibility and sensitivity to gender issues</i>
<i>Team work</i>	<i>Criticism and self-criticism</i>
<i>Working in an international environment</i>	<i>Production of free, creative and inductive thinking</i>
<i>Working in an interdisciplinary environment</i>	.....
<i>Production of new research ideas</i>	<i>Others...</i>
	.....

Search, analyze and synthesize data and information, using the necessary technologies

- Teamwork
- Promoting free, creative and inductive thinking
- Adaptation to new situations

### (3) SYLLABUS

*Symmetry processes and symmetry elements. Point groups. Group theory (definition and properties of groups). Representations of point groups. Character tables. Applications of molecular symmetry. Symmetry and visual activity. Symmetry and degeneration. Symmetry and electronic transitions. UV-Vis spectra. Selection rules. Symmetry and normal vibration modes (IR and Raman Spectra). Selection rules.*

*Identify active vibrations and peaks that are visible in IR*

*Identify active vibrations and peaks that are visible in Raman*

*Determination of vibration symmetry*

### (4) TEACHING and LEARNING METHODS - EVALUATION

<b>DELIVERY</b> <i>Face-to-face, Distance learning, etc.</i>	Face-to-face	
<b>USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY</b> <i>Use of ICT in teaching, laboratory education, communication with students</i>	The use of software to simulate molecular motions and vibrations in the molecule itself, as well as the effectiveness of Gauss view in the precise way of representing vibrations enables the student to immediately understand the role of symmetry in the interpretation of vibration spectra.	
<b>TEACHING METHODS</b> <i>The manner and methods of teaching are described in detail. Lectures, seminars, laboratory practice, fieldwork, study and analysis of</i>	<b>Activity</b>	<b>Semester workload</b>
	<i>Lectures</i>	39
	<i>The student's study hours</i>	36

<i>bibliography, tutorials, placements, clinical practice, art workshop, interactive teaching, educational visits, project, essay writing, artistic creativity, etc.</i> <i>The student's study hours for each learning activity are given as well as the hours of non-directed study according to the principles of the ECTS</i>		
	Course total	75
<b>STUDENT PERFORMANCE EVALUATION</b> <i>Description of the evaluation procedure</i> <i>Language of evaluation, methods of evaluation, summative or conclusive, multiple choice questionnaires, short-answer questions, open-ended questions, problem solving, written work, essay/report, oral examination, public presentation, laboratory work, clinical examination of patient, art interpretation, other</i> <i>Specifically-defined evaluation criteria are given, and if and where they are accessible to students.</i>	<b>LANGUAGE OF EVALUATION:</b> Greek  <b>METHOD OF EVALUATION:</b>  (i) Written work (50%) (ii) Written exam at the end of the semester (50%)	

#### (5) ATTACHED BIBLIOGRAPHY

*-Suggested bibliography:*

- F. Albert Cotton, Chemical Application of Group Theory
- . K.A. Tsipis, Quantum Chemistry
- I.D. Vergados, Group Theory
- G. B. Thomas-Ross L. Finney, Threatening Calculus