

Basic/Essential Course Information	
Course title	Chemical structure
Degree Course title	Physics
ECTS	6
Compulsory attendance	Yes
Course teaching language	English

Teacher	Savino Longo	savino.longo@uniba.it
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ECTS Details	Disciplinary area/broad field:	SSD	ECTS
	Characterizing	CHIM/03	6

Time management and teaching activity type	Period	Year	lesson type
	2st semester	1rd	Lessons (40h) Laboratory (15h)

Time management,	Total hours	in-class/in-lab study hours	out-of-class study hours
	150	55	95

Course calendar	Starting date	Ending date
	1.04.2019	10.06.2019

Syllabus	
Prerequisites	Basic inorganic and organic chemistry. Theories of chemical bonding. Structure of matter.
Expected learning outcomes (according to Dublin Descriptors)	<p><b>Knowledge and understanding:</b> Using the concepts of group theory to understand physical and chemical systems.</p> <p><b>Applied knowledge and understanding:</b> The student is able to extract useful information from the character tables and apply the theory of symmetry to molecular systems / crystal.</p> <p><b>Judging autonomy:</b> Students are encouraged to choose personal solutions for the proposed problems and to propose interesting study cases that can be the essential part of the exam interview.</p> <p><b>Communicative Skills:</b> Know how to expose the particularities of case</p>

	<p>studies and propose solution techniques, discussion in the classroom is encouraged</p> <p><b>Learning Skills:</b> Know how to extract operational information for case studies from formal texts.</p>
Course contents summary	Use of the theory of symmetry, and in particular the character tables of the punctual groups, to discuss molecular orbitals and IR/Raman spectra of isolated molecules and solids. Propose and evaluate structural models for molecules and crystals,
<b>detailed syllabus</b>	Recall of the VSEPR method and the Molecular Orbital (MO) Method. Huckel's method and secular determinant. How to build up a structural model. Computational methods. Operations and elements of molecular symmetry. Groups of symmetry operations. Representations of point groups and character tables. Orbital and vibrational symmetry modes. IR / Raman Selection Rules: traditional method. Correlation method, descending and ascending correlations. Site symmetry and multiplicity of a site. Correlation tables. Crystal tables for site groups. Case study applications: isolated molecules and some examples of crystalline solids.
books	<p>Fateley, W. G., Dollish, F. R., McDevitt, N. T., &amp; Bentley, F. F. (1972). Infrared and Raman selection rules for molecular and lattice vibrations. <i>Viley: New York</i>.</p> <p>Harris, Daniel C., and Michael D. Bertolucci. <i>Symmetry and spectroscopy: an introduction to vibrational and electronic spectroscopy</i>. Courier Corporation, 1978.</p>
notes	Some chapters
Teaching methods	Lessons with proposal and discussion of cases of study. Guided analysis of made-available tables.
<b>Assessment</b> % of final mark	Results of the final presentation (50%), presentation and discussion (50%)
Evaluation criteria	<p>the student</p> <ul style="list-style-type: none"> <li>• <b>knows</b> the principles of group theory and their application to chemical structure</li> <li>• <b>knows</b> how to evaluate structural models for molecules and crystals</li> <li>• <b>knows</b> the main method for the production of quantitative data in structural chemistry</li> <li>• <b>knows how to use</b> characters tables and correlation tables</li> <li>• <b>knows how to realize</b> a presentation.</li> <li>• <b>knows how to present</b> the results of a structural analysis in written and oral forms;</li> </ul>
other	