Faculty of Sciences

CHIM2292   Complements of groups theory and strutural chemistry

[22.5h+0h exercises] 2.5 credits

This course is not taught in 2006-2007
This course is taught in the 2nd semester

Teacher(s):	Jean-Paul Declercq
Language:	French
Level:	Second cycle

Main themes

1. Complements of group theory and chemical applications : function space and transformation operators ; equivalent representations ; the great orthogonality theorem ; construction of character tables ; projection operators ; direct product of representations ; vanisching integrals ; molecular vibrations : symmetry of the ground state and of the fundamental levels, assigning of normal modes by the projection operator ; construction of hybrid orbitals, molecular orbitals symmetry; qualitative energy diagrams; correlation tables ; application of the symmetry to chemical reactions.
2. Aspects of structural chemistry : empiric methods of molecular modelling : energy minimizing, conformational space exploration , molecular dynamics, molecular graphics ; complements of crystallography : exploitation of crystallographic databases, resolution and refinement of structures, small angle X-ray scattering and characterization of polymers.

Other information (prerequisite, evaluation (assessment methods), course materials recommended readings, ...)

Prerequisites: introduction to symmetry (CHIM1241A: Crystallography).
Evaluation: oral examination with written preparation.

Other credits in programs

CHIM22	Deuxième licence en sciences chimiques	(2.5 credits)