

[22.5h+0h exercises] 2.5 credits

This course is taught in the 2nd semester

**Teacher(s):** Jean-Paul Declercq  
**Language:** french  
**Level:** 2nd cycle course

**Main themes**

1. Compléments 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 ; vanishing 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 credits in programs**

**CHIM22** Deuxième licence en sciences chimiques (2.5 credits)