

**CHIM2181 Quantum chemistry I**

[22.5h+0h exercises] 2 credits

This course is not taught in 2006-2007

This course is taught in the 1st semester

Teacher(s): Daniel Peeters**Language:** French**Level:** Second cycle**Aims**

This course aims to initiate the chemistry students to the elementary notions of quantitative chemistry and to their application in problems encountered by chemists. It does not refrain itself to a formal teaching, but also includes an initiation to the practice of the discipline.

Main themes

Introduction to the formalism of quantum chemistry. Presentation of mono and multi configuration methods followed by their use in the calculation of structural, electronic and energetic molecular properties, and in the determination of reaction mechanisms.

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

Prerequisites: general chemistry and basics in molecular physical chemistry (CHIM1180).

Evaluation: written examination.

Support: detailed plan of the course and reference books.

Other credits in programs

CHIM22 Deuxième licence en sciences chimiques (2 credits)