

CHE 498 DIRECTED RESEARCH
Fall 2005
Marian College
3200 Cold Spring Road, Indianapolis IN 46222

**Theme: Research in Molecular Spectroscopy and Applied
Quantum Chemistry**

Instructor: Dr. Roderick M. Macrae
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Office Hours: MWF 10.30-12.00 am R 2.00-4.00 pm
Lecture: TBA
Laboratory: TBA (2-3 semester hours total)

Course Description: This course provides the opportunity for students with strong chemistry background and skills to carry out laboratory or computational research on a topic chosen by agreement with a faculty member, perform appropriate literature searches related to their chosen topic, analyze data, and report their findings through an ACS-style manuscript and a formal oral presentation.

Textbooks: No required textbook. Suggested supplementary texts include

Exploring Chemistry with Electronic Structure Methods, by James B. Foresman and Æleen Frisch (Gaussian Inc.)

Computational Chemistry, by Guy H. Grant and W. Graham Richards (Oxford Chemistry Primers, 1995)

(and others available in the laboratory)

Other needs: Hardbound laboratory notebook (available in bookstore)

Scientific calculator

Course Summary and Objectives:

On successful completion of CHE 499 a student should be able:

- To demonstrate a practical understanding of the principles of the scientific method.
- To demonstrate abilities in quantitative reasoning and calculation, and in analytical reasoning and interpretation of numerical data.
- To demonstrate scholarship and dedication to the study of chemistry.
- To show an openness to scientific criticism and to think and argue critically.
- To carry out research and use literature in an ethical manner.
- To demonstrate skill in laboratory and library research.
- To maintain proper research notebooks.
- To write professional reports.
- To demonstrate communication skills in written and oral presentations for an expert and non-expert audience.
- To demonstrate a satisfactory level of computer literacy.
- To demonstrate the ability to plan and systematically carry out a series of experiments or calculations to study a particular problem in chemistry.

Project description:

Project 1: Spectroscopy of I₂ and polyiodide ions.

Project 2: Emission spectroscopy of AA flames – search for interferent effects of complex anions.

Project 3: Factors influencing hydrogen bonding in DNA base pairs.

(Or others to be selected by consultation with instructor.)

Course Requirements and Assessment Method:

- The student must read and digest all necessary background material.
- Thorough literature searches using both online and other methods must be used as required throughout the project.
- All proposed research activities must be discussed thoroughly with the instructor in advance.

- The research must be conducted in a suitably diligent and careful manner.
- Appropriate safety measures must be taken in all procedures.
- The student must attend all group meetings and be prepared to discuss the current state of progress of his/her research project.
- A comprehensive written report must be submitted to and accepted by the instructor by the end of the semester.
- An oral presentation must be given in a forum approved by the instructor (or, alternatively, an oral or poster presentation must be given in a forum outside Marian College).
- You are expected to understand and adhere to the College's policy on academic honesty as outlined in the Marian College *Code of Student Rights*.
(<http://www.marian.edu/forms/studentcodebook.pdf>).

Attendance:

Weekly attendance of all CHE 498 B students at group meetings is mandatory, and a suitable number of hours per week are expected to be spent in the laboratory, library, or elsewhere on campus working on the project.

Grading Criteria:

A letter grade will be assigned on the basis of completion of the course requirements based on the scheme: A – excellent performance; B – good performance; C – acceptable performance; D – marginal performance; F – unacceptable performance.