

**CHE 498 DIRECTED RESEARCH**  
**Spring 2007**  
**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 10.00-10.50 am R 2.00-4.00 pm  
Lecture: TBA  
Laboratory: TBA (2-4 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 (depending on research area) include

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

*Essentials of Computational Chemistry – Theories and  
Models*, 2<sup>nd</sup>. Ed., by Christopher J. Cramer (Wiley  
2004) (available in bookstore)

(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 498 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 the ability 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.

## Description of current projects:

Project 1: Spectroscopic and computational studies of I<sub>2</sub> and polyiodide ions and their host-guest complexes with polysaccharides.

Project 2: Emission spectroscopy of flames – study of combustion intermediates, reaction kinetics, and spectroscopic thermometry.

Project 3: Computational and FT-IR/isotopic substitution studies of hydrogen bonding in DNA base pairs.

Project 4: Spectroscopic studies and stochastic kinetic modeling of oscillating reactions.

Project 5: Polymethine dyes – aggregates, excited states and photochemical reaction products.

Project 6: The chemistry of hydrogen isotopes, including muonium.

(Other projects may 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 (approximately 3 per credit hour) 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.

Calendar – important dates:

January 19 – abstract deadline for MESCON, University of Evansville. (See <http://csserver.evansville.edu/mescon> for details.)

February 23 – registration/abstract deadline for Butler University Undergraduate Research Conference.  
(See <http://www.butler.edu/urc> for details.)

March 31 – Mathematics, Engineering and Science Undergraduate Research Conference (MESCON), University of Evansville.

April 10 – Marian College Undergraduate Research Symposium in Chemistry.

April 13 – Undergraduate Research Conference, Butler University.