

Syllabus CH 443, 543
Computational Chemistry (Mathematical Methods for Chemists)

Fall Quarter, 2007
Department of Chemistry
Portland State University

Professor: Albert S. Benight, Ph.D.

301b- SB1, Office Hours: T, TH, 3:00-4:00 (or by appointment)
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Textbook: Mathematical Methods for Scientists and Engineers. McQuarrie: 978-1-891389-24-5

Prerequisites: College physics and calculus, general and physical chemistry

Homework: Problems will be routinely assigned, collected and graded. Worked out solutions to some of the homework problems will be provided. Homework will account for 5% of the final grade.

Two Midterm Examinations: Test mastery of mathematical concepts and applications presented and studied in homework exercises. No makeup exams will be given, if you miss a midterm, the other one will count towards your grade.

Final Examination: Comprehensive over all material: Tuesday Dec 4, 12:30-2:20 PM

Grading: 5% homework; 30% each midterm; 40% final examination

Summary

The focus of this course is to provide advanced undergraduates and graduate students in chemistry a practical survey of the basic mathematical techniques routinely employed in physical chemistry. General mathematical methods and constructs will be introduced; demonstrated utility will be achieved through practical physical chemistry applications. Topics include: functional integrals and integral transforms; complex analysis; multivariable and vector calculus; differential equations; and mathematical statistics.