

CHEMISTRY 52
SPRING 2001

Group Theory, Quantum Chemistry, and Spectroscopy
Prof. Karukstis

Chemistry 52 is the second course in the Physical Chemistry sequence at Harvey Mudd. This course provides a quantitative interpretation of the microscopic world through the study of group theory, quantum chemistry, and spectroscopy. Topics will include (but are not limited to): groups, symmetry elements and operations; group multiplication tables; generators, point groups, subgroups, conjugates, classes; matrix representation of symmetry operations; reducible & irreducible representations; character tables; normal modes of vibration, vibrational spectroscopy selection rules; quantum mechanical principles; particle-in-a-box and simple harmonic oscillator models; single-electron and multi-electron atomic emission spectra; s, p, and d wavefunctions; term symbols; Hund's rules, Zeeman effect; electronic spectra of polyatomic species; symmetry of molecular orbitals; molecular term symbols; rotational spectroscopy; vibrational-rotational spectroscopy.

CLASS MEETINGS: Class meetings are scheduled at 10:00 a.m. on Mondays, Wednesdays, and Fridays in Jacobs B134. Daily attendance at class is expected and participation in course discussions and exercises will be assessed.

TEXTS: We will use two texts this semester: (1) Daniel C. Harris and Michael D. Bertolucci, Symmetry and Spectroscopy, Dover Publications, NY, 1989, and (2) P. W. Atkins, Physical Chemistry, Sixth Edition, WH Freeman, 1998, Chapters 11-17. Reading assignments will be given for each class.

COURSE WEB SITE: A daily schedule of class topics and reading assignments will be posted on the course web site at <http://www2.hmc.edu/~karukstis/chem52s2001/chem52s2001.htm>. The page may also be accessed through the HMC Course Web Page listing or the Chemistry Department web page - select Curriculum - Home Pages.

OUT-OF-CLASS ASSIGNMENTS: Daily assignments will be distributed in class and are designed to correlate with the class material and the course texts. These assignments are selected to extend your understanding of concepts as well as details of calculations. Some problems will be assigned as individual assignments to be submitted once at a specified time. For other assigned problems, a group of typically three students will be selected to present the solutions in class. The group will meet outside of class, prepare a written key to the problems to distribute to all members of the class, and prepare overhead transparencies of the solutions. One or more members of the group will be selected by the instructor to present the solutions to the class. The group will receive an overall score on their solutions and presentation, so it is important for every member of the group to understand each solution. The composition of the groups will be chosen by the instructor and may be re-assigned during the semester. If a group member is not in attendance when solutions are presented in class, the instructor has the discretion to not award points to that group member.

IN-CLASS EXERCISES: During some class meetings random or assigned groups will be asked to prepare a solution to specific questions in class. On some occasions, scores will be awarded to the group's solution. Scores on a series of such in-class exercises will be summed and counted as a question on an upcoming quiz.

QUIZZES: Five quizzes have been scheduled at periodic intervals throughout the semester. Generally these quizzes will be held in class for 30 - 50 minutes, but, depending on the subject matter and time constraints, some of these quizzes may be given as take-home assignments with a longer duration. Quizzes have been scheduled (in consultation with Chemistry 56) for Wednesday **January 31**, Wednesday **February 21**, Wednesday **March 7**, Friday **March 30**, and Wednesday **April 18**.

FINAL EXAMINATION: The final exam will be given as a take-home exam due for seniors on Friday, May 4 at 5:00 p.m. and due for all others on Thursday, May 10 at 11:00 a.m.

COURSE EVALUTION: Grade . Quizzes (50%) + Final Exam (20%) + Individual Homework and Out-of-Class Group Assignments & Presentations (30%)

INSTRUCTOR'S OFFICE: My office location is Jacobs 1220- Please come by! If you would like to arrange a specific appointment, please see me, send an e-mail message, or call x73225. Best wishes for an enjoyable semester!

TENTATIVE SCHEDULE:

Monday	Wednesday	Friday
Jan 15 No Class	Jan 17 Course Begins	Jan 19
Jan 22	Jan 24	Jan 26
Jan 29	Jan 31 Quiz #1	Feb 2
Feb 5	Feb 7	Feb 9
Feb 12	Feb 14	Feb 16
Feb 19	Feb 21 Quiz #2	Feb 23
Feb 26	Feb 28	Mar 2
Mar 5	Mar 7 Quiz #3	Mar 9
Mar 12 SPRING BREAK	Mar 14 SPRING BREAK	Mar 16 SPRING BREAK
Mar 19	Mar 21	Mar 23
Mar 26	Mar 28	Mar 30 Quiz #4
Apr 2 No Class - ACS Mtg	Apr 4	Apr 6
Apr 9	Apr 11	Apr 13
Apr 16	Apr 18 Quiz #5	Apr 20
Apr 23 Presentation Days	Apr 25 Presentation Days	Apr 27
Apr 30	May 2 Classes End	May 4 Final Exam - Seniors
Thursday, May 10 - Final Exam Due 11 a.m.		