CHEM270: Math, Computer and Other Practical Skills of Chemists

Instructor: Dr. Karl Sohlberg
               Office: 222 Disque Hall.
               Email: kws24@drexel.edu
               Office hours MW 14:00-15:00, also by appointment or drop-in.

Where: Korman 111F

When: MWF 15:00-15:50

Text: There is none. Dr. Sohlberg will make handouts available electronically.

Prerequisite: successful completion of general chemistry or equivalent. (Additionally, fluency with the use of the Windows OS is expected.)

The purpose of this class is to help students of chemistry and related disciplines build a variety of skills that are valuable for a professional chemist. It should be equally applicable to biologists, physicists, chemical engineers, materials engineers etc. In particular, this class will cover:
- how to represent chemical problems in mathematical language
- how to use software like Maple and Excel to solve problems that arise in chemistry
- how to use software for the processing, analysis and graphical presentation of data
- how to use software like Hyperchem and Molkel to visualize and analyze molecular structures
- the American Chemical Society guidelines for professionalism in chemistry

To develop skills in these areas, students will be given practice with example problems (homework). An effort will be made to use chemical examples throughout the course to highlight the relevance of the skills being studied to chemistry.

Grading: There will be five components to the course grade.
1) Five quizzes each worth 10% (50%)
2) preparation of a scientific graphic and its oral presentation, 10%
3) oral "defense" of a dubious case of chemist conduct, 10%
4) Final exam, 30%.
5) The instructor may call upon you to present your solution to a homework problem in class. If done correctly and properly presented, this will earn +2% to your cumulative course average.

In the event of a missed quiz, the final exam will count 40% of the overall course grade.

The final letter grade for the course will be determined according to the following scale:
90.00-92.99, 93.00-97.99, 98.00-100 are A-, A, A+, respectively.
80.00-82.99, 83.00-86.99, 87.00-89.99 are B-, B, B+, respectively.
70.00-72.99, 73.00-76.99, 77.00-79.99 are C-, C, C+, respectively.
0.00-59.99, 60.00-66.99, 67.00-69.99 are F, D, D+, respectively.
The instructor reserves the right to lower, but not raise, the letter grade thresholds, but in no case will a score of less than 50% result in a passing grade for the class.

Syllabus as of 27 February 2014. Tentative and subject to change at discretion of instructor.

Notes about grading:
1. The grading standard will be very high. There is no substitute for the right answer. Dropping a minus sign, use of incompatible units, missing by one decimal place, dividing when you should have multiplied; these are not minor oversights, they are wrong. Some of you will eventually be in jobs where people will die if your calculations are off by a factor of ten. Make a habit of getting the right answer.
2. When work is turned in it must be submitted by e-mail as a single ***.PDF** file unless *explicitly* directed otherwise by the instructor.
3. Work turned in late but less than 1 week overdue will be graded and the score multiplied by 0.75. Late work more than 1 week overdue will be graded and the score multiplied by 0.5.
4. Attendance is expected and may influence the "instructor's discretionary component" of the final letter grades.

Adherence to university computer usage policy is expected. Violations of this policy will be dealt with at the greatest level of severity allowed under university policy.

Software: You will need to use several different software packages in this course, including:
- Stuff you probably already have:
    - **MS Word**
    - **PowerPoint**

- Stuff you will need immediately:
    - **Excel**
    - **Maple**

- Stuff you will need later in the term:
    - From Drexel
        - **Acrobat** (or equivalent, to create PDF files, any turned-in assignment must be submitted by e-mail as *.PDF.)
        - **Hyperchem** (Can be used in Koman classroom or Disque 406; some students have successfully used it over VPN but this is unsupported.)
    - Free on the internet
        - **Molekel** (http://molekel.cscs.ch/wiki/pmwiki.php)
        - **GetData** (http://getdata-graph-digitizer.com/index.php). It is free for a 21-day trial period, so don't install it until you are going to use it.

Much of the software is installed on the classroom commuters or is available for download from the Drexel software distribution site: http://www.drexel.edu/irt/software/

Items in **blue** are freely available on the internet at the web addresses shown.

IMPORTANT NOTE: *The on-line lectures posted to the course web site are intended only as a supplement to the classroom lectures. These on-line lectures were developed several years ago for an on-line version of the course. They are now partially obsolete, but many students still find them useful so they are posted as supplementary material. Do not rely on these as a primary source of course content.*

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Tentative schedule:

- Week 1: (1-6, 1-8, 1-10)
    - 1 Intro, syllabus, grading etc.
    - 2 univariate equations
    - 3 computer lab
- Week 2: (1-13, 1-15, 1-17)
    - 1 computer lab
    - 2 quiz univariate equations
    - 3 simultaneous linear equations
- Week 3: (1-22, 1-24)
    - 1 Monday no class
    - 2 oops - snow day!
    - 3 simultaneous nonlinear equations
- Week 4: (1-27, 1-29, 1-31)
    - 1 computer lab
    - 2 quiz simultaneous equations
    - 3 using N points to determine an $(N-1)^{th}$ degree polynomial, linear least-squares fitting, polynomial least-squares fitting, linearization of non-linear data
- Week 5: (2-3, 2-5, 2-7)
    - 1 general least-squares fitting, why least-squares and not least absolute error, general optimization problems.
    - 2 computer lab
    - 3 quiz curve fitting
- Week 6: (2-10, 2-12, 2-14)
    - 1 numerical differentiation and integration
    - 2 digitization of data
    - 3 How a molecule is represented computationally, construction and analysis of molecular structures
- Week 7: (2-17, 2-19, 2-21)
    - 1 computer lab
    - 2 computer lab
    - 3 quiz derivatives and integrals
- Week 8: (2-24, 2-26, 2-28)
    - 1 Graphics: scatter plots, histograms, axis scaling, axis breaks, tic marks and labels, multiple ordinates, error bars, use of colors
    - 2 Graphics
    - 3 computer lab
- Week 9: (3-3, 3-5, 3-7)
    - 1 quiz molecular structures, graphics
    - 2 Graphic due as PDF by e-mail to Dr. Sohlberg Tuesday 23:59.
    - 3 discuss readings, copyright transfer agreement, guidelines for referees , "similar" passages from scientific papers, "similar" figures in papers
    - 4 discuss readings
- Week 10: (3-10, 3-12, 3-14)
    - 5 defenses
    - 6 defenses
    - 7 defenses
- Week 11: (3-17)
    - 1 catch-up day or review (FE TBA)

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