Computational Science Program for Ohio Community and Technical Colleges

Draft Competencies for Introduction to Computational Chemistry
March 2008

Unit I: Data Analysis
This entire unit is a mastery topic and should be considered review (~1 to 1.5 weeks). According to Bloom's Taxonomy, this unit should be ranked at "Analysis" (level 4).

Topics to be covered:

- Review significant figures and the rules governing the use of sig figs in measurements
- Review the difference between systematic and random error
- Review the difference between precision and accuracy
- Review the difference between (and be able to calculate) absolute and relative uncertainty
- Review how to calculate:
    - The arithmetic mean
    - The standard deviation
    - The confidence interval (using the Student's t)
    - The Q Test to determine if a set of data is "bad"
    - Generate a calibration curve using the method of least squares

Computational Laboratory topics could include:

- Use a statistical package to calculate x-ray diffraction data for copper and perform statistical analysis on the data (Sime, 6-17 and 153-160)

Unit II: Kinetics
The anticipated unit will start from topics introduced in general chemistry and work towards more challenging topics. The individual topics are classified according to Bloom's taxonomy. (2-3 week)

Topics to be covered:

- How are rates determined and measured (application)
- Be able to determine a rate law and calculate/determine the rate constant and overall order of reaction (application)
- Be able to use the Arrhenius equation to explain how temperature influences a chemical reaction (application)
- Be able to explain how a reaction mechanism is derived from a rate law and apply it to S_N2 and S_N1 reactions (comprehension)
- Introduce the steady-state approximation (knowledge)
- Be able to apply kinetics in order to understand (knowledge)
    - Molecular motion in liquids (Fick's first and second laws of diffusion)
    - Molecular motion across membranes
    - Ion transport through membranes (and apply it to gel electrophoresis)

    - How ion channels and ion pumps work
    - The Michaelis-Menten mechanism of enzyme catalysis

Computational Laboratory work could include:

- Be able to understand a biochemical reaction (Tyrosine → DOPA → Dopachrome) by studying the enzyme used in the reaction (Tyrosinase)
    - Determine the concentration of tyrosinase in an unknown concentration by UV-Vis spectroscopy
    - Determine the proper concentration of tyrosinase necessary to use for a kinetic assay
    - Determine the kinetic parameters (K_M, V_{max}, and k_{cat}) by making a Michaelis-Menten plot and a Lineweaver-Burk plot

- Using Swiss-PDB Viewer to study the protein chymotrypsin
    - Determine how to view alpha-helices and beta-pleated sheets
    - Determine what are the hydrophilic and hydrophobic parts of the molecule
    - Display the active site of the protein
    - Investigate the function of the molecule
    - Propose a mechanism of how chymotrypsin hydrolyzes peptide bonds

Unit III: Gases

The anticipated unit will start from topics introduced in general chemistry and work towards more challenging topics. The individual topics are classified according to Bloom's taxonomy. (1.5 to 2 weeks)

Topics to be covered:

- What is a state function? (knowledge)
- What is the ideal gas law and how was it derived? (comprehension)
- Explain Dalton's Law of Partial Pressures (comprehension)
- Be able to explain and derive the kinetic-molecular theory of gases (comprehension)
- Be able to show how the van der Waals equation is an approximation to "real-life" gases (knowledge)
- Be able to calculate the Boltzmann Distribution for a given set of data (knowledge)

Computational Laboratory topics could include:

- Calculate the Lennard-Jones potential between 2 Hydrogen, Methane, Oxygen, and Chlorine atoms/molecules
- Show how the van der Waals equation of state is a better approximation to "real-life" gases as compared to the ideal gas law
- Model one-dimensional and three-dimensional gases in order to view the distribution of velocities, and probability densities.

Unit IV: Thermodynamics

The anticipated unit will start from topics introduced in general chemistry and work towards more challenging topics. The individual topics are classified according to Bloom's taxonomy. (3 to 4 weeks)

Topics to be covered:

- Be able to define the following: system, surroundings, exothermic process, endothermic process (application)
- Be able to state and explain the three laws of thermodynamics (comprehension)
- Be able to define what is meant by enthalpy and how it relates to the heat capacity (comprehension)
- Be able to explain what a phase is and a phase transition (comprehension)
- Be able to apply Hess' law to find the overall enthalpy for a certain reaction (comprehension)
- Be able to define entropy in terms of an isothermal expansion of an ideal gas and heating a system of constant heat capacity (knowledge)
- Be able to define the Gibbs' Free-Energy and explain how it changes with pressure and temperature (knowledge)
- Introduce collision theory and to be able to set up a function that determines the forces involved in a chemical reaction (knowledge)
- Introduce the concepts of potential energy and energy minimalization in a system (knowledge)
- Explain how the Gibbs energy can be used to help "predict" how biomolecules assemble (proteins, nucleic acids, phospholipid bilayer) (knowledge)

Computational Laboratory work could include:

- Determine the heat capacity of silver
- Determine the heat capacity of iodine
- Determine the vapor pressures of benzene and chloroform

Unit V: Quantum Mechanics

The anticipated unit will most likely be new material to students and would be classified as "knowledge" on Bloom's taxonomy. (4-6 weeks)

Topics to be covered:

- Define what blackbody radiation is and how it is described mathematically and how it is related to the Planck Distribution
- State the photoelectric effect and how it confirms the wave-particle duality
- Be able to state and explain Bohr's theory of the hydrogen atom and what assumptions were made about it
- State the explain the Heisenburg Uncertainty Principle and be able to show how it works for a small particle (a photon) as compared to a large particle (a baseball)
- State the Schrodinger equation and be able to describe all variables used in the equation
- Be able to solve the Schrodinger equation to the 1-D particle in a box
- Be able to describe the phenomena of tunneling

- Be able to show how the 2- and 3-D solution for the particle in a box problem is obtained
- Be able to state the 4 main postulates of quantum mechanics?
- Describe how the quantum mechanical harmonic oscillator leads to a definite solution to the hydrogen atom
- Be able to explain how approximations are used to model other many-electron atoms
- Introduce students to the Born-Oppenheimer Approximation and how it is used in quantum mechanics and programs like Spartan
- Explain the advantages and disadvantages to Valence Bond (VB) and Molecular Orbital (MO) theories
- Introduce spectroscopy and how it is used in chemistry
  - Absorption, IR, Raman, NMR?

Computational Laboratory work could include:

- Use computational tools to:
  - explore Planck's Distribution of Wavelengths
  - determine the best length of the H_2^+ ion.
  - prepare a rotational spectrum of HCl
  - prepare an infrared spectrum of HCl
- Use computational tools to:
  - prepare plots of R_{1s}, R^2_{1s}, and $r^2R^2_{1s}$ for the hydrogen atom
  - plot hydrogen atom angular wave functions in two dimensions (p_z; d_{xz})
  - solve the 2-D particle in the box problem using 3-D plots
  - prepare a 3-D parametric surface plot of a $2p_x$ orbital
- Use Spartan to [molecular mechanics]
  - Determine the conformation of n-butane that is most stable (and minimized energy)
  - Compare the chair and boat conformations of cyclohexane and determine the most stable configuration (by looking at bond lengths, bond angles, etc)
  - Compare and contrast cis- and trans-2-butene in energy; which has the lowest energy?
- Use Spartan to [ab initio / semiempirical methods]
  - Calculate heats of formation by using the AM1 method and compare values when looking at isomerism, tautomerism, and regioselectivity
  - Calculate heats of formation by using the AM1 method of the reactant, possible carbocations, and products of four compounds (methyl bromide, ethyl bromide, isopropyl bromide, and t-butyl bromide) and determine the order of reactivity of each
    - Determine the effects of solvation of the ions
  - Prepare an density-electrostatic potential map (EMP) of acetic, chloroacetic, and trichloroacetic acid and compare the acidities of each compound, as well as the electron densities around each of the carbonyl groups

    - Prepare a density-electrostatic potential map (EMP) of methyl, ethyl, isopropyl, and t-butyl carbocations and determine if the positive charge is localized in the same place on all compounds.
    - Prepare a density-electrostatic potential map (EMP) of allyl and benzyl carbocations; how is the charge distribution different in each carbocation?
    - Prepare a density-LUMO map of acetone, 2-cyclohexanone and norboranone and determine where the reactive sites are in each compound.

Unit VI: Statistical Mechanics – to be introduced if time permits

Topics to be covered:

- Be able to use the Boltzmann Distribution
- What is the partition function and what does it indicate?
- Be able to define and explain each part of the molecular partition function
- What is the Boltzmann Distribution formula for entropy?
- How are G and K_{eq} related to the Boltzmann Distribution?