Content

(15 Jan) First day of class. Hydrogen isotope exchange. Review of Mathematica.

Attached Files: thermo_syllabus2018.pdf (209.575 KB)
01Intro_H2D2.nb (116.323 KB)

Learning goals:

- Discuss course expectations
- Introduce a statistical approach to chemical reactions: The H_2/D_2 isotope exchange reaction
- Review of Mathematica: Variables, lists, associations, functions.

Readings:

- Syllabus
- Review ICPC Appendix A

(16 Jan) Review of molecular energy levels: Atoms and Diatomic Molecules

Attached Files: 02Quantum_Review.nb (17.224 KB)

Learning Goals:

- Review the quantized energy levels of atoms and diatomic molecules (covered in PChem I)
  - Electronic energies of the hydrogen atom
  - Electronic energies in general
  - Particle-in-a-Box model for translational energy
  - Quantum Harmonic Oscillator model for vibrations of diatomic molecules
  - Quantum Rigid Rotator model for the rotations of diatomic molecules
- Understand scaling changes of these energies with respect to changes in molecular properties (e.g., atomic masses, bond length, bond strength) and external parameters (e.g., confining potentials)

Readings:

- McQ 1.1-1.8 [Warning: Watch out for the difference between ν (Greek *nu*) and v . (Roman *vee*) int he equations for the harmonic oscillator. Can you appreciate why I prefer expressing these as $\hbar \omega$?]
- ICPC Appendix C (up to and including C.4.1)

(18 Jan) Mathematical Review: Conceptual Calculus

Attached Files: 03Calculus_Review.pdf (175.708 KB)

Learning Goals:

- Review differentiation and integration of single and multi-variable functions
- Review series expansion

Readings:

- McQ Math Chapter C—This is a review from last semester
- McQ Math Chapter D

Note: This does not play a role in this week's computational essay, but is laying the ground work for the coming weeks.

(22 Jan) Gas Laws and Equations of State

Attached Files: 04GasLaws_v2.nb (28.877 KB)

Learning goals:

- Review the ideal gas law (equation of state)—discuss intensive and extensive unit systems
- Introduce the compressibility, *Z*—discuss notion of departure functions
- Introduction to cubic equations of state (van der Waals, Redlich-Kwong, Peng-Robinson)
- Strategies for solving cubic equations

Readings:

- McQ 2.1-2.2
- ICPC 10.1-10.3

(23 Jan) Learning from experimental data

Attached Files: 05_GasLawData_v2.nb (66.985 KB)
Latour 21-DRAWING-THINGS-TOGETHER-GB.pdf (381.98 KB)

Learning goals:

- Acquire strategies for data representation and regression. Application to gas measurements.
- Practice model fitting as a means of extracting chemical insight from experimental data. Application to determining the nature and magnitude of intermolecular interactions of gas phase molecules

Readings:

- ICPC Appendix B

Supplementary Readings (mentioned in class):

- Bruno Latour biography (wikipedia)
- Latour's article on Writing and Cognition (graphs = science) posted above (pdf)

(25 Jan) Liquid-vapor phases; Law of Corresponding States

Attached Files: 06_IsothermsCoexistenceCriticalpoint.nb (7.994 MB)

Learning goals:

- Use vocabulary of: isotherm, coexistence curve, critical point, reduced parameter
- Model liquid-vapor phases using cubic equations of state
- Law of corresponding states
- Introduce virial equation of state

Readings:

- McQ 2.3-2.4.
- Just *skim* McQ 2.5-2.6. The main point is that there is a rigorous, quantitative theory for assigning the constants you fit to intermolecular interactions. However, it will take us several weeks before you will know why eq (2.25) (and its descendants) are true.

(29 Jan) Review of quantized energies in polyatomic molecules & Computational MO theory

[No class meeting today—please study this on your own; I encourage you to work in pairs]

Learning Goals:

- Review of vibrational and rotational energy levels in polyatomic molecules
- Review of the use of WebMO calculation to compute electronic, vibrational, and rotational energy levels for arbitrary molecules

Readings:

- McQ 1.9-1.11
- Review ICPC Appendix C
- Read ICPC Appendix D

WebMO Access:

- Log in via http://54.147.239.120:1841
- Username = your email user name (e.g., jschrier)
- Password = your student ID (e.g., "A14...") . — please change this after log in—please let me know by email if you are locked out.
- **Test your understanding** by computing the relevant information for species in the Water gas shift, Haber-Bosch process, or phosgene synthesis (relevant to this week's computational essay)

(30 Jan) Review of Symbolic and Numerical Calculus in Mathematica

[No class meeting today; please review this material on your own. I encourage you to work in groups]

Learning Goals:

- Review of symbolic and numerical calculus operations in Mathematica

Readings:

- ICPC 10.4 (but, what I really suggest is reading the entirety of ICPC Chapter 10)

Test your understanding:

- ICPC Problem 10-3, 10-4, 10-13
- ICPC Problem 10-6

Supplementary Reading:

- Mathematica's "How to: Calculus" https://reference.wolfram.com/language/howto/DoCalculus.html

(01 Feb) A review of probability; Introduction to the Boltzmann Factor

Attached Files: 03A_Probability.pdf (2.725 MB)

[We will start the class with a short guest lecture by Dr. James Lockhart of Brookhaven National Laboratory]

[Please note: This class is in JMH 404]

Learning Goals:

- Review of fundamental aspects of probability and statistics
- Conceptual motivations for and introduction to the Boltzmann distribution

Reading:

- McQ B
- McQ 3.1

Supplementary material:

I've uploaded a "mini-lecture" reviewing probability. This should be familiar from quantum chemistry last Fall...in fact, it is even easier because there are no wavefunctions, and we need only work with the probabilities or probability densities directly.

(05 Feb) Introducing the "Partition function"

Attached Files: 10BoltzmannCalculations.nb (139.796 KB)
06b_CommentOnBoyleTemperature.nb (51.572 KB)

Learning Goals:

- Introduction to the partition function (normalization factor)
- Computing derived properties from the partition function

Readings:

- McQ Chpt 3-1 to 3-5—start from the beginning to get the "flow" of the chapter
- Please note: McQ makes many "deferred promises" in this discussion (e.g., what particular partition functions are). Takes his word on them for now. The goal is to practice some of the basic derivative operations.
- Also note: Don't get too hung up on the partition function as a "magical" entity. Computing any of the average properties could also be done by summing over states, as demonstrated in the Mathematica notebook.

Practice problems (to help you think through the mathematics...try these by hand):

- McQ 3-2 (try this by hand...practice with logarithmic properties
- McQ 3-16

(06 Feb) More on partition functions

[We will start the class JMH 140 with a guest lecture by Dr. Sung Joon Kim, Howard University]

Learning Goals:

- Identify (independent & distinguishable) versus (independent & indistinguishable) chemical systems...and derive general expressions for their respective partition functions.
- Distinguish between bosonic and fermionic partition functions
- Decompose molecular partition functions into degrees of freedom

Readings:

- McQ 3-6 to 3-8

Practice problems:

- McQ 3-22 (do this by hand; useful mathematical practice for manipulating summations)
- McQ 3-32 (i.e., based on knowledge of the partition function, derive Dalton's Law of Partial Pressures)

(08 Feb) Translational, electronic, and vibrational partition functions of ideal diatomic gases

Learning goals:

- Apply your knowledge of partition functions and the quantized energy levels of atoms and molecules to calculate the translational, electronic, and vibrational partition functions for ideal (i.e., non-interacting) gases.
- Use relative magnitudes to decide appropriate approximations when performing derivations
- Evaluate thermodynamic properties of interest (e.g., average energy, pressure, heat capacity) for ideal monoatomic gases

Readings: McQ 4.1 - 4.4

Practice problem: McQ 4-10

(12 Feb) . Rotational partition functions. Molecular partition function

[We will start the class with a guest lecture by Dr. Elizabeth Thrall of Harvard University]

[Meeting in JMH 404]

Learning Goals:

- Calculate the rotational partition function for diatomic and polyatomic molecules, taking proper account of molecular symmetry properties
- Combine the partition functions for the different degrees of freedom to obtain the molecular partition function, and apply this to calculate heat capacity of diatomic gases.

Readings:

- Review McQ 4.3 and then continue to read McQ 4.5-4.9
- (You'll notice that McQ 4.8 is essentially a recap of the earlier readings, but with polyatomic molecules. The math is the same, just more tedious because the summations go over more variables. Be sure to work through the derivation of the rotational partition function in McQ 4.5 with a pencil in your hand, to make sure you understand it.

(13 Feb) Introduction to Metropolis Monte Carlo Sampling

Learning Goals:

- Consider ways of approximating functions using random sampling
- Introduction to the Metropolis Monte Carlo (MMC) sampling method
- Application of MMC to toy examples with single degrees of freedom.

Readings:

- ICPC Section 9.1.1—the classic example of using random sampling to estimate a quantity
- ICPC Chapter 11— feel free to skip Section 11.2.2 on a first reading

Practice problem: ICPC 11-4 — this is your first example of a problem with interacting degrees of freedom (here the variables *x* and *y*)

Big picture: Monte Carlo methods are widely used in finance, epidemiology, and statistical inference (machine learning) in addition to molecular simulations. (You can even use them to solve the Schrödinger equation; see ICPC Chapter 9)

(15 Feb) Heat, Work, and Internal Energy

Learning goal:

- A return to the the "macro-world" of thermodynamic laboratory measurements...
- Formal definition of "heat" and "work"

- Distinguish between "reversible" and "irreversible" processes
- Perform calculations involving pressure-volume work and heat
- Application of the concept of "state functions" to thermodynamic problems
- State and apply the First Law of Thermodynamics (in terms of internal energy, heat, and work) to thermodynamic problems of gases

Readings:

- McQ 5.1-5.3
- (review Math Chapter D on partial derivatives)

Pre-class query: In your own words (based on your reading), how would you define:

- Reversible/Irreversible process
- Isothermal
- Temperature
- Heat
- Work
- Temperature
- First Law of Thermodynamics (as an equation)

Practice problems:

- McQ D-6
- McQ 5-1, 5-2, 5-4, 5-8 (derive the equations "by hand'" to get used to the conceptual manipulations. The relevant integrands are simple polynomials and you should do these by hand as well. Feel free to perform the final numerical calculation in Mathematica though.

(19 Feb) NO CLASS TODAY—Monday Schedule

Reminder: Classes at FCRH follow a "Monday" schedule today.

(20 Feb) Adiabatic processes; Microscopic interpretations of heat and work

Learning Goals:

- Introduction to adiabatic processes
- Define "heat" and "work" in terms of microscopic energy levels and populations
- Definition of Enthalpy

Reading: McQ 5.4-5.7

In your own words...what is?:

- Adiabatic process
- Explain heat and work microscopically and macroscopically
- Enthalpy

Practice problems: McQ 5-15, 5-19, 5-21 (again, for the purposes of learning, work these out by hand to get a feel for the thermodynamics

(22 Feb) Practical calculations with Enthalpy

Learning Goals:

- Understand and apply enthalpy changes
- Calculate heat capacity under constant volume and constant pressure condition
- Use tabulated data on heats of reaction and heat capacity to compute enthalpy changes for chemical reactions

Readings: McQ 5.8-12

Practice problems:

- McQ 5-37, 5-39, 5-40, 5-48
- For the Mathematically inclined: 5-27
- Apropos your laboratory experiments: McQ 5-52

(26 Feb) Entropy and the Second Law

Learning goals:

- Macroscopic definition of "entropy"
- State and apply the Second Law of Thermodynamics to determine spontaneity of processes

Readings:

- McQ 6.1-6.4 & 6.6 (that's right, skip McQ 6.5 for now)

Practice problems:

- McQ 6-13 (Hint: for a constant pressure process what is dq_{rev}> How might this relate to enthalpy and heat capacity?)
- McQ 6-18, 6-19 (Hint: Don't overthink these problems; it's just like Gen Chem)

(27 Feb) Entropy: Microscopic definition and applications

Learning Goals:

- Apply the Binomial distribution and Stirling's approximation to problems in statistical thermodynamics.
- Understand and apply microscopic/statistical definitions of entropy
- Introduction to the Carnot Cycle

Readings:

- McQ Math Chapter E
- McQ 6.5-6.9

Practice Problems:

- McQ 6-20, 6-35, 6-36 (short mathematical derivations; do these by hand to get a feel for the logic)
- McQ 6-29, 6-45 (short numerical calculations; plots generated in Mathematica would look nice)

(01 Mar) The Third Law of Thermodynamics

Learning Goals:

- State and apply the Third Law of Thermodynamics
- Qualitative rationalization and quantitative calculation of entropy changes with changing temperature, pressure, and volume
- Continued practice of application of entropy state function calculation to chemical reaction problems
- Qualitative rationalization of standard molar entropies and residual entropy in terms of molecular structure and energy levels.

Readings: McQ Chapter 7 (all)

In your own words...:

- How does entropy change with increasing temperature?
- What's the Third Law of Thermodynamics?
- Rank these gases in terms of their standard enthalpy: chloroform, carbon tetrachloride, helium. Explain your ranking in terms of microscopic molecular energy levels.
- Which of those molecules might have a residual entropy? Why?

Practice problems:

- McQ 7-7, 7-9 (very short pencil-and-paper derivations; be sure to do this so you can grasp the logic)
- McQ 7-41, 7-42 (qualitative assessments; you should do these on sight without detailed calculation)
- McQ 7-48 (short calculation, like you did in gen chem)
- McQ 7-35 (define a short Mathematica function to compute the partition functions; combined with the enthalpy difference, what insight does this give you into the equilibrium constant of the H_2/D_2 isotope exchange reaction?)

(05 Mar) Introduction to the Helmholtz and Gibbs Energies

Learning goals:

- Introduce new state functions corresponding to experimentally-convenient situations (specifically: Helmholtz energy and Gibbs energy) and apply them to chemical problems
- Introduction to the Maxwell Relations

Readings: McQ 8.1-8.4

Practice problems:

- McQ 8-1, 8-2 (the former is just a Gen Chem problem; the latter requires you to do a little calculus to incorporate the heat capacity information into your value for the entropy change)

(06 Mar) More Gibbs Energy

Learning goals:

- Apply the Maxwell relations to transform thermodynamic expressions to different conditions (T, P)
- Use *fugacity* to describe non-ideal behavior of thermodynamic systems

Readings: McQ 8.5-8.8

Practice Problems:

- McQ 8-43, 8-44 (these are literally just a matter of following along the instructions in the problem using a pencil and paper. I would derive these for you in class, but it is more valuable for you to try. Don't overthink these...just follow the algebra as directed by McQ.
- Apropos: you might take a look at 8-48 and 8-50, as it relates to laboratory

(08 Mar) Phase equilibria

Learning Goals:

- Interpret phase diagrams
- Use Gibbs Energy to understand solid-liquid-gas equilibria
- Introduce the concept of chemical potential (Gibbs energy per particle)
- Construct qualitative G(T) curves using knowledge of microscopic energy levels and use them to reason about chemical processes

Reading: McQ 9.1-9.3

Practice problems: McQ 9-1, 9-17, 9-36

(12 Mar) . Pressure dependence of phase transitions

Attached Files: Physics Today 2005 Rosenberg.pdf (384.422 KB)

Learning goals:

- Apply the Clausius-Clapeyron equation to study vapor pressure changes
- Evaluation of the chemical potential from atomic and molecular partition function

Readings:

- McQ 9.4-9.5

Practice problems:

- McQ 9-28, 9-37

Supplementary reading:

- "Why is Ice Slippery?" (Physics Today 2005 Rosenberg)

(13 Mar) Microscopic models of phase transitions: The 2D Ising Model

Learning Goals:

- Introduce the 2D Ising model as a model for phase transitions of interacting systems and use Monte Carlo simulations to observe phase behavior

Readings:

- ICPC 12.1-12.3 . (be sure to get the code working)

Questions to test your understanding...

- In your own words, how might a model like this might be used to describe a phase transition? How might it be used to describe a solute in a solution? Explain the meaning of J and B parameters in terms of chemical bonds and/or chemical potentials.

Practice problem: (you will work on this in class) . ICPC 12-5

(15 Mar) Generalizations and Applications of the Ising Model

Learning Goals:

- Introduce the concept of periodic boundary conditions, it's thermodynamic applications, and computational implementation,
- Generalize the Metropolis algorithm to conserve particle numbers
- Application of the Ising model to illustrate general principles of phase transitions

Readings:

- ICPC 12.4
- ICPC 13.1-2

In your own words...

- What are some example problems where the use of periodic boundary conditions is an appropriate treatment? Inappropriate treatment?
- What's a thermodynamic problem where it is necessary to conserve particle numbers of a given type?

Practice problems:

- Pick one of ICPC 13-2, 13-3, 13-4, or 13-5 and implement it.

Preview:

- After Spring break, we'll be looking at the thermodynamics of solutions. If you are interested, you can look at ICPC 13.3 as a preview.

SPRING BREAK

No classes during Spring Break.

(26 Mar) Introduction to Liquid-Liquid Solutions

Learning Goals:

- Study of liquid-liquid (miscible in all proportions) solutions.
- Introduction to the use of partial molar quantities in thermodynamic calculations
- Introduction to the Gibbs-Duhem equation
- Ideal solutions and Raolt's Law
- Distillation as a thermodynamic process
- Construction of vapor-liquid coexistence curves

Readings:

- McQ 10.1 - 10.4

Practice problems

- McQ 10-20, 10-21 (Hint: Generate Table[]s of {x1,t} and {y1,t} values using P1 and P2 as inputs, then ListPlot[] the result to generate the temperature-composition diagram.

(27 Mar) . Non-ideal solution thermodynamics

Learning goals:

- Extend the thermodynamic theory of solutions to non-ideal solutions
- Discuss properties of temperature-composition and liquid-vapor diagrams for non-ideal solutions
- Introduction of "activity" as a thermodynamic quantity and practical calculations
- Introduction to the regular solution theory

Readings:

- McQ 10.5 - 10.9

Practice Problems:

- McQ 10-37, 10-44

(29 Mar) Solid-liquid solutions

Learning goals:

- Introduction to the thermodynamic theory of ideal Solid-liquid (not miscible in all proportions) solutions
- Review of Raolt's Law, Henrys Law, and Colligative properties, and their thermodynamic oriigin
- Review of freezing point depression, boiling point elevation, and osmotic pressure

Reading:

- McQ 11.1-11.4

Test your understanding. Without referring to any notes (i.e., from memory) can you explain and write equations for...?:

- Raolt's law
- Henry's Law
- Freezing point depression, boiling point elevation, and osmotic pressure
- What are the conditions for being an ideal solution? What types of chemical systems would you expect to be <u>non</u>-ideal solutions?

Practice problems: (There are all short numerical calculations, similar to those you did in Gen Chem. It is expected that every chemistry major can do these without difficulty.)

- McQ 11-3, 11-26, 11-29, 11-32

(02 Apr) Electrolyte solutions. Intro to Chemical Equilibrium

Learning goals:

- Properties of (non-ideal) electrolyte solutions
- Physical motivations of the Debye-Hückel theory
- Introduction to chemical equilibrium as a Gibbs Energy minimization problem

Readings:

- McQ 11.5-11.7 (just skim over the derivation of the Debye-Hückel theory; in general this only works well for very dilute solutions; in practice one uses empirical departure functions to describe the system)
- McQ 12.1-12.2 (use Mathematica to make your own version of Fig 12.1)

Practice problems: (again, short problems that every chemist should be able to carry out...)

- 11-32, 11-43, 11-44
- 12-6 (there is no specific numerical value of the equilibrium constant to use. Instead the gal is to derive a simple formula, similar to the one shown int he text of problem 12-3 at the top of the page)

(03 Apr) A closer look at equilibrium

Learning goals:

- Use the Gibbs energy to peunderstand and perform practical calculations invovling chemical equilibria
- Use "activities" to correctly predit equilibria in non-ideal systems.
- Relate equilibrium constants to other thermodynamic variables and molecular partition functions

Reading:

- McQ 12.3 - 12.8. If you have time, go back to the beginning of the chapter and read it again.

Practice Problems that all chemists should be able to do:

- McQ 12-8, 12-9, 12-17, 12-29* (don't over think this...the polynomial expression makes this a simple exercise)
- Pick one of the following: 12-20, 12-22

(05 Apr) More equilibrium

Learning Goals

- Use JANAF thermodynamic tables to perform equilibrium calculations
- Use "activities" to correctly predict equilibria in non-ideal systems

Readings:

- McQ 12.8 -12.12

Reference Material:

- NIST-JANAF Thermochemical Tables https://janaf.nist.gov/

Practice problems:

- McQ 12-44, 12-61, 12-63

(09 Apr) Intro to Electrochemistry

Learning Goals:

- Gain familiarity with the terminology and notation used for describing electrochemical cells
- Thermodynamics of electrochemical processes

Readings:

- McQ 13.1-13.6

(10 Apr) Applied electrochemistry

Learning Goals:

- Application of electrochemistry to determine thermochemical properties of interest (e.g., activity coefficients, reaction entropies and enthalpies, solubility products, weak acid dissociation constants)
- Discussion of fuel cells

Readings:

- McQ 13.7-13.11

(12 Apr) Introduction to the Kinetic Theory of Gases

Availability: Item is not available. It will be available after Mar 25, 2019 11:59 PM.

Attached Files: McQuarrie_and_Simon_Physical_Chemistry_Chapter_27.pdf (9.878 MB)

Learning Goals:

- Derivation of the kinetic theory of gases from the Boltzmann distribution
- Could the ancient Greeks/Romans/Indians have discovered the ideal gas law and the Boltzmann distribution?
- A turn towards molecular processes in time.

Readings:

- Physical Chemistry: A Molecular Approach (PC:AMA) Chapter 27.1-27.4
- (download attached PDF)

Supplementary Reading:

- A brief overview on *De rerum natura* https://en.wikipedia.org/wiki/De_rerum_natura
- English translation of *De rerum natura* http://classics.mit.edu/Carus/nature_things.html
- Philosophical atomism in the Classical Greek tradition https://plato.stanford.edu/entries/atomism-ancient/
- Philosophical atomism in the Classical Indian tradition https://plato.stanford.edu/entries/naturalism-india/#IndConNat
- Atomism in the modern period (17th-20th Century) https://plato.stanford.edu/entries/atomism-modern/

(16 Apr) Gas-gas collisions as a theory of chemical reaction rates

Availability: Item is not available. It will be available after Mar 25, 2019 11:00 AM.

Attached Files: McQuarrie_and_Simon_Physical_Chemistry_Chapter_27.pdf (9.878 MB)

Learning Goals:

- Derive expressions for the collision frequencies, mean free path between collisions, and reactive collision rates from the kinetic theory of gases.

- Use these expressions as a model for gas-phase chemical reaction rates

Readings: PC:AMA 27.5-27.7 (attached PDF)

(17 Apr) Chemical Kinetics

Availability: Item is not available. It will be available after Mar 25, 2019 11:00 AM.

Attached Files: McQuarrie_and_Simon_Physical_Chemistry_Chapter_28.pdf (11.86 MB)

Learning Goals:

- Review of chemical reaction kinetics and rate law derivations.
- Note: These should be familiar to you from general chemistry. Please be sure that you can derive the integrated rate laws for the basic reactions.

Readings: PC:AMA 28.1-5 (attached)

Practice problems: PC:AMA 28-10 (no sophisticated calculations are needed!) , 28-19

(19 Apr) NO CLASS — Good Friday

Availability: Item is not available. It will be available after Mar 25, 2019 11:00 AM.

There are no classes today at FCRH. (Good Friday)

(23 Apr) Chemical Kinetics: Relaxation methods and Temperature Dependence of Rate Constants

Availability: Item is not available. It will be available after Apr 1, 2019 11:55 AM.

Attached Files: J Chem Educ 1972 LAIDLER.pdf (1.289 MB)
McQuarrie_and_Simon_Physical_Chemistry_Chapter_28.pdf (11.86 MB)

Learning Goals:

- Apply your knowledge of chemical reaction kinetics to compose experiments for determining rate constants (e.g., relaxation methods).
- Introduction to the Arrhenius model for the temperature-dependence of rate constants (and its interpretation from kinetic collision theory)

Readings: PC:AMA 28.6-28.7 (attached PDF)

Supplementary reading: I've attached a supplementary reading on unconventional (i.e., non-chemical) applications of the Arrhenius Law, which is quite amusing to read.

(24 Apr) Chemical Kinetics: Reaction Mechanisms

Availability: Item is not available. It will be available after Apr 1, 2019 11:05 AM.

Attached Files: McQuarrie_and_Simon_Physical_Chemistry_Chapter_29.pdf (13.866 MB)

Learning Goals:

- Construct chemical reaction processes out of elementary reactions
- Apply common approximations (e.g., steady state approximation, initial rates, fast equilibrium) to obtain approximate analytical solutions to sets of coupled differential equations.

Readings:

- PC:AMA 29.1-5 (download PDF attached)

Practice problems:

- PC:AMA 29-9, 29-11

(26 Apr) Numerical Methods in Chemical Kinetics

Availability: Item is not available. It will be available after Apr 1, 2019 11:30 AM.
Attached Files: McQuarrie_and_Simon_Physical_Chemistry_Chapter_29.pdf (13.866 MB)

Learning Goals:

- Introduction to numerical differential equation integration to solve chemical kinetics problems
- Review of classic model reaction mechanics: Lindemann Unimolecular decay, Michaelis-Menten Equations

Readings:

- ICPC 15.1
- PC:AMA 29.6-9 (pdf attached)

(30 Apr) Stochastic kinetics

Availability: Item is not available. It will be available after Apr 8, 2019 4:09 PM.

Learning goals:

- Extension of chemical kinetics to problems involving small numbers of molecules, and consequences in nanotechnology and biology
- Kinetic Monte Carlo methods for solving stochastic kinetics problems

Readings: ICPC 15.2-3

(01 May) Transition State Theory

Availability: Item is not available. It will be available after Apr 8, 2019 4:16 PM.
Attached Files: Mini Lecture 26A_Transition State Theory.pdf (5.113 MB)
Worksheet: TST_PES.docx (616.521 KB)
Galano 2006 J Chem Educ.pdf (262.749 KB)
Wang 2014 Nature Chem - Nanoreactor.pdf (1.835 MB)

Learning Goals:

- Derive and understand the transition state theory of chemical reaction rates
- Apply transition state theory to simple cases
- Interpretation of potential energy surfaces

Readings: PC:AMA Section 28.8 (pdf attached)

Mini Lectures: Please watch the (~20 min) pencast mini lecture.

Supplementary reading: The readings and mini-lecture only describe how to compute the rates in a general way. The paper by Galano *et al.* (linked above) shows in more explicit detail how to use quantum chemistry calculations (e.g., using QWebMO) to obtain chemical reaction rates via transition state theory, with a specific application to atmospheric chemistry. Doing this in WebMO is (at least in principle) easy—just **optimize for the transition state**! —but in practice this can be challenging to identify the coordinates. Alternatively, one can just watch the reactions occur in real time by performing molecular dynamics simulations using the Born-Oppenheimer potential determined by quantum chemistry calculations. See the article by Wang et al (linked above) for a particularly stunning example of this type of direct "nanoreactor" simulation for determining chemical rates.

FINALLY: Please take 10 minutes to complete the SEEQ

(07 May) FINAL EXAM (G-Block)

Availability: Item is not available. It will be available after Apr 1, 2019 4:42 PM.

The Final Exam is tentatively assigned to Tuesday, 07 May at 9:30am