Introduction to Physical Chemistry
Chemistry 59-240 - Fall 2012 v. 12

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Teaching Assts.	Frank, Guerrero, Hirsh, Li, Lucier & Veinberg
Office Hours:	***By appointment only*** - **please use the contact page** to schedule a time slot
Lectures:	MWF 12:30-1:20, 104 Toldo
Tutorials:	See schedule on web, 4 sessions
Labs:	See schedule on web, 5 labs

Update: Sept. 7, 2012; p. 1; modified overall content

Course Materials
Chemistry 59-240

Textbooks:

1. Atkins, P.W. and De Paula, J. Physical Chemistry, 9th edition. Vol. 1: Thermo-dynamics and Kinetics, W.H. Freeman, 2011, ISBN 1-4292-3127-0.
2. Trapp, C, Cady, M. and Guinta, C. Students Solution Manual for Physical Chemistry for 9th edition, W.H. Freeman, 2011, ISBN 1-4292-3128-9.

*****8th edition of Atkins will also be supported!***

Miscellaneous:

1. Scientific Calculator
2. Web access: http://chem240.cs.uwindsor.ca
   New site! Should be complete on weekend!

Grading System
Chemistry 59-240

Mark Breakdown:

Mid-term 1	20%	Wed., Oct. 17, 2012
Mid-term 2	20%	Fri., Nov. 16, 2012
Lab	15%	
Final Exam	45%	Wed., Dec. 12, 2012

Letter Grades:

93-100	A+	87-92.9	A	80-86.9	A-
76-79.9	B+	73-75.9	B	70-72.9	B-
66-69.9	C+	63-65.9	C	60-62.9	C-
56-59.9	D+	53-55.9	D	50-52.9	D-
36-49.9	F	0-35.9	F-		

Intro Week
Chemistry 59-240

Intro Week:

- Takes place in **235 Essex Hall** beginning the week of Monday, September 10th, 2012.

- If you are regularly scheduled at 2:30, show up at your normal day and time.
- If you are regularly scheduled at 6:00, show up on your normal day, but at 3:00 p.m.

- Meet your TAs
- Get assigned lab partners and schedules
- Review safety regulations
- Become familiar with the lab

- Lab manuals: available on CLEW site - be sure to bring a copy of the manual along with you!!

Course Motivation
Chemistry 59-240

Physical Chemistry: Quantitative and theoretical study of the properties and structure of matter, and their relation to the interaction of matter with energy.

■ This course serves as an introduction to ***chemical thermodynamics***, giving you an understanding of basic principles, laws and theories of physical chemistry the are necessary for chemistry, biochemistry, pre-medical, general science and engineering students.

■ You will develop the ability to solve ***quantitative problems***, and learn to use original thought and logic in the solution of problems and derivation of equations.

■ You will learn to apply mathematics in chemistry in such a way that the equations paint a ***clear picture*** of the physical phenomena

Course Outline
Chemistry 59-240

We will cover most of **Chapters 1-5** of "*Physical Chemistry*" by P.W. Atkins (9th edition)

0. Introduction to Physical Chemistry
1. The properties of gases
2. The First Law
3. The Second Law
4. Physical transformations of pure substances
5. Simple mixtures
17. Surface tension (handouts from new book)

Course Outline
Chemistry 59-240

We will cover most of **Chapters 1-6** of "*Physical Chemistry*" by P.W. Atkins (8th edition)

0. Introduction to Physical Chemistry
1. The Properties of Gases.
2. The First Law of Thermodynamics
3. The Second Law of Thermodynamics: Concepts
4. Physical Transformations of Pure Substances
5. Simple Mixtures
6. Phase Diagrams

Studying Physical Chemistry †

Hints on how to study in physical chemistry courses

- ***Summarize*** each set of notes on one page in an organized form that helps to isolate all key points: “nerd notes”
- ***Download*** all available handouts, including equation sheets
- Start working on problems with the ***equation sheets*** a.s.a.p. and do not fall behind
- Physical Chemistry is not a “memory-based”, learn-by-rote discipline, but is centred upon ***problem-based learning***. However, you must practice solving problems, deriving equations, etc. to become proficient.
- Review ***assigned*** and ***in-class problems***
- Try the A/B list problems with your solutions manual
- Attempt the corresponding B/A list problems
- Attend ***tutorials***
- View ***animations*** and use other web resources
- Book consultation times **after** you have attempted a majority of the problems

What is Physical Chemistry?

Physical chemistry includes numerous disciplines:

Thermodynamics - relationship between energy interconversion by materials, and the molecular properties

Kinetics - rates of chemical processes

Quantum Mechanics - phenomena at the molecular level

Statistical Mechanics - relationships between individual molecules and bulk properties of matter

Spectroscopy - non-destructive interaction of light (energy) and matter, in order to study chemical structure

Photochemistry - interaction of light and matter with the intent of coherently altering molecular structure

Physical Chemistry @ UWindsor

What courses are available in Physical Chemistry?

- ☐ 59-240: Thermodynamics: Physical & Chemical Properties of Materials
- ☐ 59-241: Kinetics, Statistical Thermodynamics & Reactions
- ☐ 59-340: Quantum Chemistry - Properties of Molecules
- ☐ 59-341: Symmetry & Spectroscopy - Interaction of Light and Matter
- ☐ 59-351: Materials Chemistry - Physical Inorganic Chemistry

Honours/Graduate Level

- ☐ 59-440: Photochemistry & Kinetics
- ☐ 59-441/541: Statistical Mechanics
- ☐ 59-445/542: Nuclear Magnetic Resonance (NMR) Spectroscopy
- ☐ 59-470/570: Computational Chemistry & Molecular Orbital Theory
- ☐ 59-636: Mesomorphic Materials & Polymers

Major Considerations in Phys. Chem.

- **Matter**
- **Quantifying Matter**
  - SI vs. cgs units
  - SI derived units
- **Energy**
  - Types of energy
  - Equipartition of energy
- **Quantization of Energy**
  - Energy states and populations
  - Boltzmann distributions
- **Light**
  - Dual nature: wave vs. particle
  - Wave behaviour
  - Energy of radiation
  - Relationships between matter and light

Matter

Matter: composed of electrons and nuclei (neutrons and protons) - which can be further divided into subatomic particles

Physical Properties:

mass
largely due to the nuclei; thermal properties

electric charge
atoms and molecules are bound together by **electrostatic** interactions

magnetism
nucleus interacts with magnetic fields;
little consequence for atomic or molecular structure

spin
least “tangible” property; closest classical analogy: electrons and nuclei are spinning like little planets

Quantifying Matter

Substance: A pure form of matter

Amount of substance: Reported in terms of *moles*
1 mol of a substance contains as many entities as exactly 12 g of carbon-12 (ca. 6.02×10^{23} objects)

Avogadro's Number: $N_A = 6.02 \times 10^{23}$ mol^{-1}

Extensive Property: Dependent upon the amount of matter in the substance (e.g., mass & volume)

Intensive Property: Independent of the amount of matter in a substance (e.g., mass density, pressure and temperature)

Molar Property: X_m, an extensive property divided by the amount of substance, n: $X_m = X/n$

Molar Concentration: "Molarity" moles of solute dissolved in litres of solvent: 1.0 M = 1.0 mol L^{-1}

SI vs. Gaussian Units

Units: Standards for comparison
SI: Systeme Internationale (mks - the World)
Gaussian: centimetres, grams and seconds (cgs, U.S.A.)

SI system: All quantities can be expressed in terms of seven base units:

Base quantity	Name	Symbol
length	meter	m
mass	kilogram	kg
time	second	s
electric current	ampere	A
thermodynamic temperature	kelvin	K
amount of substance	mole	mol
luminous intensity	candela	cd

for more info: http://physics.nist.gov/cuu/Units/

SI vs. Gaussian Units, 2

Older literature sources and many Americans still use the cgs system of units, so it is useful to understand the relationship between the SI and cgs systems.

SI or mks units		**Gaussian or cgs units**		
Name	**Symbol**	**Name**	**Symbol**	**Conversion**
meter	m	centimeter	cm	0.01 m
kilogram	kg	gram	g	0.001 kg
second	s	second	s	
ampere	A	biot	Bi	10 A
kelvin	K	kelvin	K	
mole	mol	mole	mol	
candela	cd	stilb	sb	10^4 cd m^{-2}

SI Derived Units

Many important units, some with special names and symbols, can be derived from the SI base units:

Derived quantity	Name	Symbol
volume	cubic meter	m^3 *or* L *or* dm^3
speed, velocity	meter per second	m/s
acceleration	m. per s. squared	m/s^2 *or* $m\ s^{-2}$
wave number	reciprocal meter	m^{-1}
mass density	kg per cubic m	kg/m^3 *or* $kg\ m^{-3}$
frequency	hertz	Hz : s^{-1}
force	newton	N : $kg \cdot m \cdot s^{-2}$
pressure, stress	pascal	Pa : N/m^2 : $kg \cdot m^{-1} \cdot s^{-2}$
energy, work, heat	joule	J : $N \cdot m$: $kg \cdot m^2 \cdot s^{-2}$
power, radiant flux	watt	W : J/s : $kg \cdot m^2 \cdot s^{-3}$
electric charge	coulomb	C : $A \cdot s$
electric potential	volt	V : W/A : $kg \cdot m^2 \cdot s^{-3} \cdot A^{-1}$
magnetic field	tesla	T: A/m

SI vs. Gaussian Derived Units

Many important units, some with special names and symbols, can be derived from the SI base units:

Derived quantity	Symbol	Conversion
erg (energy)	erg	1 erg = 10^{-7} J
dyne (force)	dyn	1 dyn = 10^{-5} N
gauss (magnetic field)	G, Gs	1 G = 10^{-4} T
Other units		
calorie (energy, thermo)	cal	1 cal = 4.184 J
calorie (food energy)	Cal	1 Cal = 1 kcal = 4184 J
electron volt (energy)*	eV	1 eV = 1.602 177 33 x 10^{-19} J
micron (distance)	μ	1 μ = 10^{-6} m = 1 μm
Angstrom (distance)	Å	1 Å = 10^{-10} m

* Energy acquired by an electron passing through a potential of 1 V in a vacuum (commonly used unit for physicists)

Energy

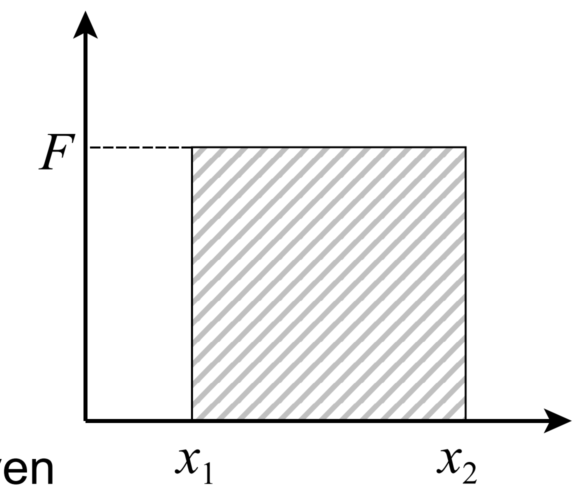
Energy: The capacity to do work (or to heat)
Work: Force causes mechanical displacement on a body

For an infinitesimal amount of work, *dw*, done by a force **F** in the *x*-direction:

$$\frac{dw}{dx} = F_x \qquad dw = F_x dx$$

$$w = \sum F(x)\,dx = \int_{x_1}^{x_2} F(x)\,dx = F(x_2 - x_1)$$

for constant F



The amount of work for finite displacement, *w*, is given by the sum of infinitesimal displacements, which is equivalent to the integral above.

Energy is conserved - it is neither created or destroyed: it can be transferred from one location to another in the form of mechanical work (orderly) or heat (thermal motion, random)

Spontaneity, Equilibria, Kinetics, etc.

Physical chemistry is about more than just defining energy:

- It's about the conversion of energy via work and heat from one source to another

- It's about why things happen and why things do not

- It is about the delicate balance between thermodynamically and kinetically allowed and forbidden processes

    Example:
    - two allotropes of carbon are diamond and graphite
    - graphite is the more thermally stable substance
    - yet, we do not observe diamonds changing into graphite
    - diamonds are said to be "kinetically stabilized"

- It's about understanding our entire universe

What about 59-240?

Thermodynamics:

Physical behaviour of solid, liquid, gas and mixed phases

Energy interconversion via **physical** (e.g., compression, expansion, mixing, heating, cooling, etc.) and **chemical** (chemical reactions, combustion, ionization, etc.) processes

1st law: “book-keeping”, making sure energy is conserved, and knowing where energy goes or comes from

2nd law: “spontaneity”, knowing why processes actually occur, why beautiful, orderly entities are created from seemingingly shear randomness

Practical applications: industrial processes, everyday phenomena, safe chemistry, understanding new materials