CHEM 231

Physical Chemistry I
NJIT
Fall Semester, 2017

Prerequisites:	**Chem 126 or 123, Phys 111**
Co requisite:	**Math 211**
Textbook:	**Peter Atkins, Julio De Paula. Physical Chemistry 10th Edition, Freeman & Co. New York, 2014**
Chapters to be covered:	**1, 2, 3, 4, 5A, 5B, 5E**
Instructor:	**Dr. Lev Krasnoperov Tiernan Hall Room 358, Phone x3592**
Goals:	**To introduce students to the basic principles of thermodynamics, Ideal and non-ideal systems, Closed and open systems, Chemical potential, Equilibrium, Phase transitions, Simple mixtures.**
Prerequisites:	**Basic chemical principles, Functions of two and several variables, Partial derivatives, Integrals.**

Course Outline:

Lecture 1, 2: Thermodynamic System. Equilibrium. State of Thermodynamic System. Zeroth Law of Thermodynamics. Ideal Gas. Boyle's Law. Charles Law. Temperature. Equation of State.

Lecture 3, 4: Importance of Boyle Temperature. Van der Waals Equation of State. Van der Waals Parameters. Critical Constants. Principle of Corresponding States. Maxwell Construction. Real Gas.

Lecture 5, 6: Energy, Work, Heat, and Internal Energy. Thermodynamics. First Law. Expansion Work. Reversible Expansion. Heat and Enthalpy. Heat Capacity.

Lecture 7: Enthalpy. Standard Enthalpy. Standard State. Enthalpy of Chemical Reaction. Standard Enthalpy of Solution, Ionization, Bond Dissociation, etc.

Lecture 8: Thermochemistry. Reference States of Elements. Standard Enthalpies of Formation. Standard Enthalpy of Formation of Ions. Temperature Dependence of Reaction Enthalpies.

First Midterm Exam

Lecture 9, 10: Thermodynamic Relations. Joule Experiment. Coefficient of Thermal Expansion. Relation between C_p and C_v. Reversibility. Entropy. Second Law of Thermodynamics. Entropy of Chemical Reaction.

Lecture 11: Adiabatic Expansion or Compression. Ideal Gas.

Lecture 12: Heat Engines. Carnot Cycle. Reversion of Heat Engines. Efficiency. Clausius Theorem.

Lecture 13, 14: Entropy of Phase Transitions. Entropy of Ideal Gas. Measurements of Entropy. Third Law of Thermodynamics. Third Law Entropies of Chemical Substances. Efficiencies of Thermal Processes.

Lecture 15: Helmholtz Free Energy. Gibbs Free Energy. Fuel Cell.

Lecture 16: Fundamental Equation. Maxwell Relations. Variation of Internal Energy with Volume. Properties of Gibbs Energy. Temperature Dependence of Gibbs Energy.

Gibbs – Helmholtz Equation. Pressure Dependence of Gibbs Energy.

Second Midterm Exam

Lecture 17: Open Systems. Chemical Potential. Pure Substances and Mixtures. Chemical Potential of Real Gases. Fugacity.

Lecture 18 - 20: Phase Transitions in Pure Compounds. Phases. Phase Diagrams. Pressure Dependence. First and Second Order Transitions. Clausius- Clapeyron Equation.

Lecture 21, 22: Properties of Simple Mixtures. Mole Fractions. Partial Molar Volume. Gibbs-Duhem Relations. Thermodynamics of Simple Mixtures. Thermodynamics of Mixing. Ideal Gas Mixture. Solutions. Colligative Properties.

Lecture 23: Binary Liquid Mixtures. Partial Vapor Pressure. Ideal Solutions. Raoult's Law. Real Solutions. Ideal Dilute Solutions. Henry's Law. Solubility of Gases.

Final Exam

Grading:

	Hour Exam 1 (after approx. 4 - 5 weeks)	**200**
	Hour Exam 2 (after approx. 8 - 9 weeks)	**200**
	Final Exam	**300**
	Homeworks[a)] (via Quizes)	**220**
	Attendance	**80**

	Total:	**1000**

Grade determination. Scores less than 45% of the total normally result in F. Scores larger than 85% of total always result in A. The distribution of the grades between these benchmarks as well as the F and A boundaries depend on the overall performance of the class.

[a)]Homework grades will be given based on THREE quizes 110 pts each, 35 min, two problems similar to those from the homework assignments, with different numerical data, TWO BEST quizes will be taken into account (homework grades will be assigned contingent submission of all homework assignments). The quizes are POP UP (i.e., are NOT announced in advance). No requests whether a quiz would appear on a specific date must be made. NO make-up quizes will be offered.

The NJIT honor code will be upheld and any violations will be brought to the immediate attention of the Dean of Students.
Students will be consulted with by the instructor and must agree to any modifications or deviations from the syllabus throughout of the semester.

Prepared: **Dr. Lev Krasnoperov**

Date: **August 16, 2017**

Learning outcomes:

By the end of the course, you should be able to do the following:

1. **Calculate pressure and molar volumes of ideal as well as real gases.**
2. **Determine the efficiency of heat engines.**
3. **Derive the basic thermodynamic relations and to state the approximations and the applicability.**
4. **Calculate the thermodynamic functions of components in pure compounds and simple mixtures.**
5. **Calculate thermodynamic functions of chemical reactions at reference as well as arbitrary temperatures.**
6. **Calculate the location of phase boundaries for pure substances.**
7. **Calculate properties of simple mixtures.**

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Homework Assignments		**Atkins, De Paula, 10 Ed.**
#1.	**Exercises:**	**1A.1(a), 1A.2(a), 1A.3(a), 1A.7(a), 1A.12(a)**
	Problems:	**1A.1, 1A.3**
#2.	**Exercises:**	**1C.4(b), 1C.7(a)**
	Problems:	**1C.2, 1C.3, 1C.7**
#3.	**Exercises:**	**2A.6(a), 2B.2(a), 2B.3(a), 2C.5(a)**
	Problem:	**2B.3**
#4.	**Exercises:**	**2A.5(a), 2C.3(b), 2C.4(a), 2C.9(a), 2C.10(a)**
	Problems:	**2A.2, 2C.7**
#5.	**Exercises:**	**2D.2(a), 2D.3(a)**
	Problems:	**2D.3, 2D.4**
#6.	**Exercises:**	**3A.11(a), 3B.2(a), 3C.2(a), 3C.3(a)**
	Problems:	**3A.7, 3A.9**
#7.	**Exercises:**	**3D.2(a), 3D.3(a), 3D.4(a)**
	Problems:	**3D.1, 3D.3**
#8.	**Exercises:**	**4A.1(a), 4B.5(a), 4B.6(a), 4B.7(a)**
	Problems:	**4B.2, 4B.3**
#9.	**Exercises:**	**4B.8(a), 4B.13(a)**
	Problems:	**4B.4, 4B.5**
#10.	**Exercises:**	**5A.7(a), 5A.9(a), 5B.3(a), 5B.5(a), 5B.7(a)**
	Problems:	
#11.	**Exercises:**	**5E.1(a), 5E.2(a), 5F.1(a), 5F.3(a)**
	Problems:	**Integrated activities 5.1**