Inter-American University of Puerto Rico
_____Campus
Department of _____

I. General Information

Course Title:	Thermodynamics
Code and Number:	**CHEM 3910**
Credits:	4 credits
Requirements:	PHYS 3002, MATH 2252,
	Concurrent CHEM 3320

Academic Term:
Professor:
Office Hours:

Office Phone:
Email:

II. Course Description:

Theoretical and experimental study of the fundamental physical principles that govern the properties and behavior of chemical systems, with emphasis on the macroscopic approach. It includes thermodynamics and its application to phase equilibriums and chemical equilibriums, non-ideal systems: real gases and solutions and electrochemistry. It requires 45 hours of conference and 45 hours of closed laboratory in person.

III. Contents:

Upon successful completion of the CHEM 3910 course, the student will have acquired the following knowledge and developed the corresponding skills:

1.   Objectives

  A.1.   Thermodynamic functions (internal energy, enthalpy, entropy, free energy, etc.) and their applications.

  A.2.   Chemical potential applied to phase equilibrium and chemical equilibrium.

  A.3.   Non-ideal systems: real gases and solutions.

  A.4.   Transport processes: thermal conductivity, viscosity, diffusion electrical conductivity.

B.1. Zero Law and First Law of Thermodynamics

B.1.1   Discuss the effect of thermodynamics and its role in chemistry-physics.

B.1.2.   Discuss the following concepts and propose examples: system and environment (surroundings); classes of systems; wall and its types; system in equilibrium and its types; thermodynamic properties and their types; states of matter and state functions; equations of state.

B.1.3.   Enunciate the Zero Law of Thermodynamics and explain its meaning. Define the concept of temperature.

B.1.4.   Establish the concept of PV type work and its mathematical expression.

B.1.5.   Distinguish between reversible and irreversible processes.

B.1.6.   Establish the concept of heat and write the mathematical expression for heat transfer between two bodies at different temperatures. Define the concepts of heat capacity and specific heat with their respective units.

B.1.7.   Write the mathematical expression for the First Law of Thermodynamics in finite terms and in differential terms. Discuss its meaning and identify the state function defined by the First Law.

B.1.8.   Distinguish between state functions and pass functions.

B.1.9.   Define the concept of enthalpy.

B.1.10   Apply the First Law to show that $U = \Delta q_V$ and that $\Delta H = q_P$

B.1.11.   Define the concepts of C_V and C_P and relate them to dU and dH.

B.1.12.   Describe Joule's experiment and define the μ_J coefficient

B.1.13.   Describe the Joule-Thomson experiment and define the μ_{JT} coefficient.

B.1.14.   Apply the First Law to perfect gas processes.

B.1.15.   Discuss reversible, isothermal, and adiabatic processes for perfect gases.

B.2. Second Law of Thermodynamics

B.2.1.   Enunciate the Second Law of Thermodynamics and explain its meaning.

B.2.2.   Describe a thermal machine and define the concept of efficiency.

B.2.3.   Discuss the Carnot principle concerning thermal machines.

B.2.4.   Describe the Carnot cycle and demonstrate that $dq/dT = 0$ for that cycle. Express the efficiency of a reversible machine in terms of the temperatures of the caloric reserves, hot and cold.

B.2.5.   Generalize that $dq/dT = 0$ for any reversible cyclic process and define the concept of entropy.

B.2.6.   Calculate ΔS for reversible, isothermal, and adiabatic processes, as well as for cyclic processes.

B.2.7.   Calculate ΔS for reversible phase changes, to constant P and T.

B.2.8.   Calculate ΔS for a reversible state change of a perfect gas.

B.2.9.   Calculate ΔS for constant heating to P.

B.2.10. Calculate ΔS for the mixture of inert perfect gases at constant P and T.

B.2.11. Determine ΔS_{univ} for reversible and irreversible processes.

B.2.12. Discuss the microscopic interpretation of entropy.

B.3 Material Balance

B.3.1.   Establish the material equilibrium condition for isolated and closed systems in terms of entropy.

B.3.2.   Define the Gibbs free energy (G) and the Helmholtz energy (A) and establish their thermodynamic meaning.

B.3.3.   Establish the material equilibrium condition in terms of quantities G and A.

B.3.4.   Identify the six basic equations of thermodynamics.

B.3.5.   Derive the expression of dU, dH, dA and dG for systems of constant composition (Gibb's equations).

B.3.6.   Apply Euler's reciprocity relation to Gibbs' equations to obtain Maxwell's relations.

B.3.7.   Define the concept of chemical potential, μ, of component "i" in a single-phase system and identify the fundamental equation of chemical thermodynamics.

B.3.8.   Establish Gibbs' equations for systems of variable composition.

B.3.9.   Understand the fundamental equation of chemical thermodynamics in a multi-phase system and identify the material equilibrium condition.

B.3.10.   Apply the general condition of material equilibrium to phase equilibrium and chemical equilibrium.

B.4   Standard Thermodynamic Functions for Chemical Reactions

B.4.1.   Define the standard thermodynamic state for pure substances.

B.4.2.   Define the concept of standard enthalpy reaction, $\Delta H^o_{rxn,T}$ and explain its meaning.

B.4.3.   Express $\Delta H^o_{rxn,T}$ in terms of $\Delta H^o_{f,,T}$ of reactants and products.

B.4.4.   Describe the pump calorimeter and discuss the energy relationships that arise in this type of calorimeter.

B.4.5.   Establish the relationship between ΔH^o and ΔU^o for a reaction between gases.

B.4.6.   Enunciate Hess's law and apply it to the calculation of $\Delta H^o_{rxn.}$

B.4.7.   Identify the expression that establishes the dependence of ΔH^o_{rxn} on temperature (Kirchoff's Law)

B.4.8.   Enunciate the Third Law of Thermodynamics, explain its meaning and apply it to the calculation of conventional absolute entropies.

B.4.9.   Define the concept of standard reaction entropy, $\Delta S^o_{rxn,T,}$ and calculate it from conventional entropies.

B.4.10.   Define the concept of Gibbs energy of reaction, $\Delta G^o_{rxn,T,}$and calculate it from the standard Gibbs' energies of formation, $\Delta G^o_{f,T.}$

B.5. Chemical Equilibrium in Gas Mixture

B.5.1.   Identify the expression for the chemical potential (μ) of a pure ideal gas at a certain temperature (T) and pressure (P).

B.5.2.   Identify the expression for the chemical potential of a gas "i" in an ideal mixture of gases at a certain temperature (T) and partial pressure (P_i)

B.5.3.   Apply the general condition of chemical equilibrium to an ideal mixture of reacting gases to establish the expression of K^o_P, the standard equilibrium constant.

B.5.4.   Set the expressions of K_c, K_x and its relation to K_P.

B.5.5   Establish the dependence of K_P on temperature and discuss the graphical method for determining ΔH^o_{rxn} from the values of K_P different temperatures.

B.5.6.   Reasonably predict the displacement of equilibrium in ideal gas mixture in a reaction by changing thermodynamic variables.

B.6.   Phase Equilibrium for Single Component System

B.6.1.   Discuss Gibbs' rule of phases and its meaning.

B.6.2.   Apply the phase rule to systems in a component and describe the phase diagram for such systems. Define the concepts of enthalpy and entropy for phase changes.

B.6.3.   Establish the Clapeyron equation and explain its meaning.

B.6.4.   Integrate the Clapeyron equation for liquid-vapor, solid-vapor, and solid-liquid equilibriums.

B.6.5.   Discuss the graphical method for determining enthalpies of vaporization and sublimation from vapor pressures at different temperatures.

B.7.   Real Gases

B.7.1.   Define the concept of compressibility factor (Z) of a real gas and establish the deviations of the ideal behavior in terms of Z.

B.7.2.   Identify the van der Waals equation and explain the meaning of its constants.

B.7.3.   Evaluate Z for a van der Waals gas and discuss the experimental curves of Z vs P.

B.7.4.   Identify the Redlich-Kwaig and virial equations.

B.8.   Solutions

B.8.1.   Define the concepts of partial molar magnitudes (V_m, U_m, H_m, S_m, G_m, etc.) of a component in a solution and explain their meaning.

B.8.2.   Express V, U, H, S, G, etc. for a solution in terms of the corresponding partial molar magnitudes of the components of the solution.

B.8.3.   Identify the expressions that define the thermodynamic magnitudes of mixture and explain their meaning.

B.8.4.   Discuss experimental methods for determining the partial molar volumes of the components of a binary solution.

B.8.5.   Define the concepts of integral heat of solution and integral heat of solution and explain their meaning. Discuss the experimental method for determining them.

B.8.6.   Establish the thermodynamic definition of ideal solution in terms of chemical potential of each component of it. Identify the standard state for each component.

B.8.7.   Determine ΔG_{mix}, ΔV_{mix}, ΔS_{mix}, ΔH_{mix} and ΔU_{mix} for an ideal solution.

B.8.8.   Derive Raoult's law from the thermodynamic definition of ideal solution and explain its meaning.

B.8.9.   Identify the mathematical expression for the vapor pressure of an ideal binary solution in terms of composition. Represent pressure versus composition for such a system.

B.8.10.   To establish the thermodynamic definition of ideally diluted solution in terms of the chemical potential of each component (solvent and solutes) of the same. Identify the standard states for the solvent and for solutes.

B.8.11.   Define Henry's law, explain its meaning and apply it to the solubility of liquid gases.

B.8.12.   Compare P vs x graphs for ideal and ideally diluted solutions.

B.9.   Non-ideal solutions

B.9.1.   Establish the thermodynamic definition of non-ideal solution in terms of the chemical potential of each component of it.

B.9.2.   Define the concepts of activity and activity coefficient. Explain its meaning.

B.9.3.   Establish Conventions I and II for non-ideal solutions in terms of standard states and coefficients of activity of the components.

B.9.4.   Define the concepts of transience and coefficient of transience of a gas in a non-ideal mixture of gases and explain their meaning.

B.9.5.   Identify the expression of the chemical potential of a gas in a non-ideal mixture of gases.

B.10.   Chemical Equilibrium for Non-Ideal Systems

B.10.1.   Derive the expression of equilibrium constant in terms of the activities, K^o, standard equilibrium constant.

B.10.2.   Apply the standard equilibrium constant to reactions in non-electrolyte solutions and set the expressions of K_x, K_c, and K_m.

B.11.   Phase Balancing for Multi-Component Systems

B.11.1   Define the concept of colligative properties.

B.11.2.   Identify the expression for the decrease in vapor pressure of a solution and explain its meaning.

B.11.3.   Set the expressions for the descent at the freezing point and the ascent at the boiling point. Explain the meaning of K_f and K_b.

B.11.4.   Define the concept of osmotic pressure and derive its mathematical expression from the phase equilibrium condition.

B.11.5.   Represent and discuss the diagrams of P vs x and T vs x for the liquid-vapor equilibrium of a two-component system that form an ideal solution.

B.11.6.   Represent and discuss the diagrams of P vs x and T vs x for the liquid-vapor equilibrium of a two-component system that form a non-ideal solution. Define the concept of azeotrope.

B.11.7.   Represent and discuss the diagram of T vs x, to P, for the solid-liquid equilibrium of a system of two miscible components in liquid phase and immiscible solid phases. Define the concept of eutectic point.

B.12.   Electrochemistry

B.12.1.   Enunciating Coulomb's Law and its Importance

B.12.2.   Define the concept of electric potential, ϕ, between two points.

B.12.3.   Establish the expression of the electrochemical potential and the phase equilibrium condition in terms of it.

B.12.4.   Describe the characteristics and main parts of a galvanic cell and an electrolytic cell.

B.12.5.   Establish the diagram of a galvanic cell given the chemical reaction involved and vice versa.

B.12.6.   Establish the half reactions on each electrode given the scheme of a cell.

B.12.7.   Apply the Nernst equation to calculate the potential of a cell.

B.12.8.   Establish the relationship between $\Delta G^o_{rxn,}$ the potential of a cell and the equilibrium constant of a redox reaction.

1.   Course Content

IV.1.   Thermodynamics

IV.1.1   Zero Law and Temperature
IV.1.2.   First Law of Thermodynamics
IV.1.3.   Second Law of Thermodynamics

IV.2.   Material Equilibrium

IV.2.1.   Gibbs and Helmholtz Free Energy
IV.2.2.   Chemical Potential
IV.2.3.   Phase Equilibrium and Chemical Equilibrium

IV.3.   Standard Thermodynamic Functions

      IV.3.1.   Standard reaction enthalpies
      IV.3.2.   Standard reaction entropy. Third Law of
                         Thermodynamics.
      IV.3.3.   Gibbs Free Energy reaction standard

IV.4.   Chemical equilibrium of a gas mixture

      IV.4.1.   Chemical potentials in ideal gas mixture
      IV.4.2.   Reaction equilibrium in ideal gas mixture
      IV.4.3.   Equilibrium constant dependence with T
      IV.4.4.   Balance shift

IV.5.   Phase equilibrium for a one-component system

      IV.5.1.   Gibbs phase rule
      IV.5.2.   Phase diagram
      IV.5.3.   Clapeyron equation

IV.6.   Real gases

      IV.6.1.   Compression factor
      IV.6.2.   Equations of state of real gases
      IV.6.3.   Real gas isotherms
      IV.6.4.   Critical condition

IV.7.   Solutions

      IV.7.1.   Partial molar amounts
      IV.7.2.   Mixing quantities
      IV.7.3.   Determination of partial molar quantities
      IV.7.4.   Ideal solutions. Raoult's Law
      IV.7.5.   Ideally diluted solutions. Henry's Law

IV.8.   Non-ideal solutions

      IV.8.1.   Activity and activity coefficients
      IV.8.2.   Determination of activity coefficients
      IV.8.3.   Electrolyte Solutions
      IV.8.4.   Debye-Huckle theory

IV.9.   Chemical equilibrium for non-ideal systems

      IV.9.1   Equilibrium constant
      IV.9.2.   Chemical equilibrium in electrolyte and non-
                         electrolyte solutions

IV.9.3.   Heterogeneous phase chemical equilibrium
IV.9.4.   Equilibrium constant dependence with T and P

IV.10.   Phase balancing for multi-component systems

IV.10.1.   Colligative properties
IV.10.2.   Decrease in vapour pressure
IV.10.3.   Descent at freezing point and ascent at boiling point
IV.10.4.   Osmotic pressure
IV.10.5.   Phase diagrams for component systems

IV.11.   Electrochemistry

IV.11.1   Thermodynamics of electrochemical systems
IV.11.2   Galvanic cells
IV.11.3   Nernst equation

1. Teaching strategies for the course:

If it is a Virtual Class:

1. The class lecture and lab will be offered virtually using the "Blackboard Collaborate Ultra" platform. The day and time of the conference and the laboratory will be those established in the course registration for the trimester.

2. To connect to the virtual class, a link has been created available on the main page of this course in Blackboard. See the following instructions:

   How to get into Blackboard:

   1. Enter the metro.inter.edu page

   2. Login to blackboard.

   3. Find the course in the list of your coursess.

   4. Enter the main page of the course and search for"Virtual Room" and click. That link will take you to the virtual class.

   5. If the student has not validated their email, they should contact Mr. Eduardo Ortiz of the CIT, at the email eortizo@metro.inter.edu

   6. If the student does not do these steps, they will not be able to access the course.

7. On the main page of the course, you will also find material that the instructor could provide such as Power Point presentations, practice exercises and internet videos. All this additional material can be included in the exams.

8. Office hours will in virtual mode on the day and time established by the instructor. You can also write your questions to the instructor using Blackboard's internal email.

If it in-person:

1. The class and the laboratory will meet in-person according to the day and time established in the course schedule

If it is by Contract:

1. The class and laboratory contract established by the Department of Natural Sciences is filled out and signed, as agreed by the instructor and students.

2. The meetings during the trimester are established. There are NO weekly meetings like a traditional class. The student will study the class material on his own and will take the exams as established previously in the contract. Some in person experiments will be conducted, and written reports of those experiments will be handed for grading.

1. **Course Evaluation:**

1. The evaluation of the course consists of two parts:

   Conference (70%) and Laboratory (30%). The following table contains the weight of each component in the conference:

Evaluation Criteria	Punctuation	Weight in the final grade (%)
Partial Exam 1	100	17.5
Partial Exam 2	100	17.5
Partial Exam 3	100	17.5
Final Exam	100	17.5
Total Points	420	70%

2. The conference includes three partial exams and a final exam of all the topics discussed in class. All exams have the same weight.

3. At the time of reviewing this syllabus (August 2021) the exams will be offered virtually and/or in person.

4. There is a final laboratory exam whose date will be announced

2. Laboratory Evaluation:

	Weight Score	in Final Grade
7 laboratory reports	700	15%
Appreciation Grade	100	3%
Final Exam Grade	100	12 %
Total Points	900	30%

1. Planned Laboratory Experiments:

1. Viscosity of an organic liquid as a function of temperature
2. Enthalpy of combustion of an organic compound
3. Partial molar volumes of aqueous solutions of NaCl
4. Conductance of strong and weak electrolytes
5. Thermodynamics of the lactone/zwitterion equilibrium in rhodamine B
6. Phase diagram of a binary system (naphthalene-p dichlorobenzene)
7. Determination of pK_a in the first excited singlet state of 2-naphthol
8. Vapor Pressure of a liquid

The lab manual has been prepared by Dr. Colom and is available on "Blackboard."

Grade scale used in CHEM 3910

The final grade of the course is calculated by adding the percent obtained in the conference (of 70%) and that obtained in the laboratory (of 30%).

100-85 A   84 - 75   B   74 - 65   C   64 – 55 D   54 - 0   F

Special Notes:

Any student who requires auxiliary services or special assistance must request them at the beginning of the course or as soon as he acquires knowledge of the services he will need, through registration in the Office of the Professional Counselor, Mr. José Rodríguez of the University Orientation Program.

Plagiarism and Fraud:

It is important to be clear that the different forms of plagiarism (the use of someone else's ideas or words without due recognition) is an academic infraction with very serious consequences. See the *General Student Regulations of the Inter-American University*

2004, from page 60 onwards for examples of the types of plagiarism and the sanctions that apply. In this course this type of practice will be penalized.

Use of electronic devices:

Cell phones and any other electronic devices that could disrupt teaching and learning processes will be deactivated. Personal situations or calls will be taken care of outside the classroom.
If you use your cell phone to "chat, watch movies, listen to music, etc." during class, I will ask you to leave the classroom or lab. The handling of electronic devices that allow access, storage or sending data during evaluations or exams is prohibited.

Course Textbook:

> Levine, I.N. "Physical Chemistry," Latest Edition, McGraw-Hill, Inc.: New York. (You can really use any of the editions.)

References:

1. Shoemaker et al., "Experiments in Physical Chemistry", 7th Edition, McGraw-Hill: New York, 2003.

2. Raff, L.M., "Principles of Physical Chemistry", Prentice Hall: Upper Saddle River, New Jersey, 2001.

3. Ball, D. "Physical Chemistry", Brooks/Cole-Thomas Learning: Pacific Gove, CA, 2003.

4. Laidler, K.J. et al., "Physical Chemistry", 4th Edition, Houghton Mifflin Company: Boston, MA, 2003.

5. Atkins, P., de Paula, J., and Keeler J. "Atkin's Physical Chemistry", 11th Edition, Oxford University Press: Oxford, United Kingdom, 2018.

6. Monk, Paul and Munro, Lindsey J. "Maths for Chemistry: A chemist's toolkit of calculations", 2nd Edition, Oxford University Press: Oxford, U.K, 2010.

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