Dublin Institute of Technology

Pre-Requisite Modules code(s)	Co-Requisite Modules code(s)	ECTS Credits	Module Code	**Module Title**
CHEM1201		5	CHEM2214	Physical Chemistry

This Header should be repeated on each page of the Module
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Module Description:
This module introduces students to fundamental concepts in kinetics, electrochemistry, thermodynamics and colligative properties as appropriate to medicinal and pharmaceutical chemistry. Emphasis will be on 'real life' context-based examples and problem solving. Students will be provided with a basis on which to study topics at a more detailed level in the third year. Laboratory experiments will complement the material covered in lectures.

Module aim:
The aim of this module is to provide the student with a basic understanding of the principles of reaction kinetics, thermodynamics, colligative properties and electrochemistry and allow them to apply this knowledge to real-world examples and laboratory experiments.

Learning Outcomes:
On completion of this module, the learner will be able to:

- Describe the principle factors governing the rate of reaction
- Describe experimental methods for determining the order and rate of reaction
- Describe electrochemical cells and the measurement of electrochemical potential
- Discuss the First Law of Thermodynamics
- Discuss experimental techniques for measuring enthalpy of reactions
- Explain the relationship between spontaneity and chemical and electrochemical processes
- Discuss the origin and application of colligative properties

Learning and Teaching Methods:
The module will be delivered encompassing a variety of learning methods. These will include lectures, formative problem-solving exercises, computer-based learning assignments, self-directed learning supported through the use of WebCT and practical laboratories.

Module content:
Kinetics
Simple collision theory. Reaction rate. Rate laws and rate constants. Reaction order. Reaction mechanisms – elementary, consecutive(Steady State), equilibrium. Integrated rate laws. Half life. Introduction to pharmacokinetics.
Temperature dependence of reaction rates. Catalysis, introduction to enzyme catalysis.
Experimental methods for studying kinetics.

Thermodynamics
Energy, First law, internal energy, heat, work. Energy systems in the body. Enthalpy, heat capacity, calorimetry, bomb calorimetry, DSC – application to thermal denaturation.Entropy and Second Law, Gibbs Free energy and spontaneity.
Phase changes, phase diagrams, polymorphism.

Electrochemistry
Redox reactions, electrochemical cells, standard potentials, Nernst equation.
Ions, ionic conductivity, ions in the body.
Membrane potentials of Neurotransmitters (Resting potential, Action potential)
Electrode sytems and sensor technology.
Electrochemical cells, metal hydride cells, fuel cells and chlor-alkali cells.

Colligative Properties
Chemical equilibrium –relating K, ΔG and E^0
Calculation of Keq
Acids and bases, pH, pOH, pK_a, pK_b, Henderson Hasselbach equation, importance of pK_a in drug design.

Buffers

The practical element of this module should cover 5 or 6 three-hour laboratories from the following:

1. Hydrolysis of Aspirin (By back titration or conductivity)
2. Determination of the reaction order and rate constant for the oxidation of iodide by persulphate in neutral solution.
3. Determination of the rate law for the iodination of acetone in acid solution.
4. Calorimetry
5. Toluene – cycloheane phase diagrams
6. Conductimetric Titrations.
7. The verification of the Nernst equation.

Module Assessment:
The student will be assessed on this module through end of module written exam and a laboratory practical module mark. The weighting between the written element, Continuous assessment and the practical element of the module is 40:20:40 respectively.

Essential Reading:
P.W. Atkins and J de Paula, Physical Chemistry for the Life Sciences, 1st Ed., Oxford University Press, 2006.
School of Chemistry, Second Year laboratory Manual.

Supplemental Reading:
H.E. Avery, (1991), Basic Reaction Kinetics and Mechanisms, Macmillan London.

Web references, journals and other:

Further Details: This module may be delivered in one semester. The contact hours may be summarised as follows; 24 hours lectures, 18 hours laboratory practical, 12 hours formative assessment/ problem solving sessions and 46 hours self study.

Date of Academic Council approval …………………………….