

The Hebrew University of Jerusalem

Syllabus

PHYSICAL CHEMISTRY A - 69163

Last update 08-04-2024

HU Credits: 4

Degree/Cycle: 1st degree (Bachelor)

Responsible Department: Chemistry

<u>Academic year:</u> 0

Semester: 2nd Semester

<u>Teaching Languages:</u> Hebrew

<u>Campus:</u> E. Safra

Course/Module Coordinator: Prof. Elad Gross

Coordinator Email: elad.gross@mail.huji.ac.il

Coordinator Office Hours: By appointment

Teaching Staff:

Prof Elad Gross, Ms. Einav Scharf, Mr. Yinon Deree

Course/Module description:

First course in the field of physical chemistry for chemistry students, which focuses on the fundamentals of physical chemistry. The guideline is a physical quantitative analysis of chemical reactions and phenomena.

The course includes quantitative treatment of gas properties and the kinetic theory of gases. In addition, it deals with chemical kinetics, i.e. the rate of chemical reactions.

The course covers definitions and basic concepts (reaction rate, rate law, reaction order, etc.), experimental measurements of reaction rates, reaction mechanisms, temperature-dependence, potential energy surfaces, etc. Applications in the fields of chemistry of the atmosphere, enzymatic reactions and photochemistry are also discussed.

<u>Course/Module aims:</u>

See Learning Outcomes.

Learning outcomes - On successful completion of this module, students should be able to:

Describe chemical phenomena in a physical approach using mathematical models.

Define and classify chemical reactions according to kinetic properties.

Know experimental methods for rate measurements and determination of reaction orders.

Know the fundamentals of the kinetic theory of gases and its application to the understanding of chemical processes in the gas phase.

Know fundamental concepts in photochemistry.

<u>Attendance requirements(%):</u> None

Teaching arrangement and method of instruction: Lecture and Exercise

Course/Module Content:

A. Mathematical Background.

B. Introduction to Chemical Kinetics.

C. Definitions and Basic Concepts:

rate of reactions, rate laws, rate constants, order of reaction (partial, full, and pseudo), reaction mechanisms, elementary and complex reactions.

D. Measuring Reaction Rates (Chemical and Physical Methods).

E. Elementary Reactions of 0,1,2,3 and n order.

Reversible (equilibrium), sequential and parallel reactions.

F. Methods for Determination of Order of Reactions.

G. Complex Reactions and Reaction Mechanisms

Assumption and approximations: rate-determining step, steady state, fast equilibrium.

H. Examples for Mechanisms:

Unimolecular Reactions & Lindemann Mechanism.

Catalysis and enzymatic catalysis – Michaelis-Menten Mechanism.

Radioactive decays.

A taste of photochemistry – Jablonski diagram, competing reactions, quantum yield, Stern-Volmer Equation.

I. Dependence of Reaction Rate of Temperature

Activation energy and reaction profile.

Arrhenius equation.

J. The Kinetic Theory of Gases:

Basic concepts and assumptions.

Maxwell-Boltzmann speed and kinetic energy distributions.

Obtaining average and most probable values.

Collision theory, cross-sections for collision and reaction, mean free path. Effusion.

Linking kinetic theory to reaction rates.

K. The Molecular Basis for Rate Constants of Reactions:

Collision theory vs. rate constants.

Potential energy surfaces (PES), reaction coordinate.

L. Transport Properties:

heat conductivity, diffusion, viscosity, diffusion-controlled reactions, mobility of ions in solution, transference numbers, ion conduction.

<u>Required Reading:</u>

Levine I., Physical Chemistry (5th Edition or later), McGraw-Hill, Boston, 2002. (QD 453.2 L49 2002)

Additional Reading Material:

Any book dealing with the basics of physical chemistry, e.g.: 1. Atkins P.W. and de-Paula J., Physical Chemistry (8th Edition or later), W.H. *Freeman, New York, 2002. (QD 453 A88 1994/1998/2002) 2.McQuarrie D.A. and Simon J.D., Physical Chemistry – a Molecular Approach, University Science Books, California, 1997*

For advanced reading: • *Levine R.D., Molecular Reaction Dynamics, Cambridge University Press, New York,* 2005. (QD 461 L66 2005)

<u>Grading Scheme:</u> Written / Oral / Practical Exam 80 % Submission assignments during the semester: Exercises / Essays / Audits / Reports / Forum / Simulation / others 20 %

Additional information:

A weekly homework exercise. Handing of at least 8 exercises. 20% of the final grade will be based upon the averaged grade of 8 exercises. Lower number of home excersies will lead to a decrease of 3 points in the final grade for each missing excersies.

Recordings will be released after two weeks.