

COURSE SYLLABUS

1. Identification

Code and title: QUP 053 – Photochemistry. Principles and Applications

Professor: Daniel Eduardo Weibel

Level: Master and Doctorate

Credit hours: 3

Revised: August_2019

2. Summary

Basic principles and applications of photochemistry in homogeneous and heterogeneous systems. Photochemical mechanisms. Physical and chemical deactivations of excited states. Photocatalysis. Photosynthesis. Laser and Synchrotron radiation. Time-resolved photochemistry.

3. Objective

Introduce students to photochemical science with an approach to the main current applications.

4. Contents

- Basic concepts in photochemistry, fundamental and excited electronic states. Light absorption and excitation sources. Excited state deactivation and Jablonski diagram. Internal conversion and system crossover. Fluorescence and phosphorescence. Lifetime of excited states. Inter and intramolecular electronic transitions. Franck-Condon principle, El-Sayed selection rules, physical and chemical quenching. Long-range energy transfer (dipole-dipole, Colombiana), short-range energy transfer. Marcus theory.
- Atmospheric and stratospheric photochemistry. Differentiate between thermal and photochemical reactions. Ozone layer. Photochemical pollution (Smog).
- Photochemistry of alkenes and carboxylic compounds. Excited state geometry. Norrish type I and II reactions. Hydrogen abstraction reactions. Primary and secondary photochemical mechanisms of decomposition. Quantum yields, deactivation, photochemical sensitization.
- Kinetic studies of transient species, Flash photolysis, Pump-probe methods: lasers. Time-resolved spectroscopy (ps and fs).
- Solar energy conversion: photovoltaic cells and dye-sensitized photovoltaic cells. Photocatalysis, artificial photosynthesis and photoelectrochemistry. Challenges in hydrogen photogeneration.
- Advanced Oxidative Processes: homogeneous and heterogeneous. Fenton-type reagents, ozone, TiO₂ and hybrid systems.
- Photochemistry on surfaces.

5. Assessment

List of exercises, presentation and discussion of scientific articles, theoretical tests and/or directed works. The student, who obtains a final grade of A, B or C, awarded as per the list below, will be considered approved:

A: grade equal to or above 9.0

B: grade equal to or above 7.5 and below 9.0

C: grade equal to or above 5.0 and below 7.5

D: grade below 5

FF: lack of frequency

6. Methodology

Lectures, exercises lists, seminars and examinations.

7. Bibliography

- B. Wardle, Principles and applications of Photochemistry, Chishester, UK, 2009, 250.
- J. N. Turro, Modern Molecular Photochemistry, The Benjamin/Cummings Publishing Company, Inc., California, 1991.
- H. Okabe, Photochemistry of Small Molecules, John Wiley & Sons, New York 1978.
- R. P. Wayne, Chemistry of Atmospheres; Oxford University Press: Oxford, 1992.
- J. G. Calvert and J. N. Pitts, Photochemistry John Wiley: New York, 1966.
- C. A. Grimes, O. K. Varghese and S. Ranjan, Light, Water, Hydrogen. The Solar Generation of Hydrogen by Water Photoelectrolysis, Springer, 2008.
- T. Oppenländer, Photochemical Purification of Water and Air: Advanced Oxidation Processes (AOPs): Principles, Reaction Mechanisms, Reactor Concepts. Weinheim, Wiley-Verlag, Germany, 2003.
- N. S. Allen, Handbook of Photochemistry and Photophysics of Polymeric Materials, John Wiley & Sons, New Jersey, Canada, 2010.
- S. Parsons, Advanced Oxidation Processes for Water and Wastewater Treatment, IWA Publishing, London, UK, 2004.
- M. Kaneko and I. Okura, Photocatalysis: Science and Technology. Tokyo, Japam, Springer, 2002.