

SC/CHEM 4024 3.00 Structure Elucidation of Organic and Organometallic Compounds

Spectroscopic methods for the identification of organic reaction products and other organic and organometallic unknowns, primarily for chemistry students. The main focus is on solving molecular structure using NMR techniques.

Offered this year in Winter term.

Three lecture hours per week. One term. Three credits.

Prerequisites SC/CHEM 3020 3.0/4.0

Text(s) & Other Materials A suggested reading list could consist of:

- Modern NMR Spectroscopy — A Guide for Chemists, 2nd ed., Jeremy K.M. Sanders, Brian K. Hunter, Oxford, 1993; ISBN 0-19-855567-9, QD 96.N8S25 1993.
- UV-Vis Spectroscopy and Its Applications, H.-H. Perkampus, Springer-Verlag, 1992; ISBN 3-540-55421-1, QD96U4P4713 1992.
- Mass Spectrometry — A Textbook, Jurgen H. Gross, Springer-Verlag, 2004; ISBN 3-540-40739-1, QD96M3G76 2004.
- Infrared Spectroscopy: Fundamentals and Applications, Barbara Scott, Wiley, 2004; ISBN 0-470-85428-6, QD96I5S76 2004.
- IR Spectroscopy: An Introduction, Helmut Gunzler, Hans-Ulrich Gremlich, Wiley-VCH, 2002; ISBN 3-527-28896-1 QD 96I5G86 2002.
- Two-Dimensional NMR Spectroscopy — Applications for Chemists and Biochemists, Eds. William R. Croasmun, Robert M.K. Carlson, VCH, 1994; ISBN 1-56081-664-3 QD96N8T87 1994.

Course Content

A course combining spectroscopy and mass spectrometry with the goal of determining structure of various types of organic and organo-metallic compounds.

- Spectroscopy overview.
- In depth presentation of key molecular and spectroscopic properties used in structural determination by NMR.
- Specific strategies will be addressed which impact on the success of these techniques.
- Description of computer programs available for spectral database searches and spectral simulation.
- Spectral properties and structural identification of sugars (and polysaccharides), natural products, aromatic hydrocarbons and organo-metallic compounds.

Chemistry 4024/5024 describes NMR spectroscopy as a comprehensive method of structure elucidation of organic and organo-metallic compounds. The course presents the theory and principles of NMR spectroscopy and introduces practical NMR experiments with interpretation of the data as a method of gaining insight into molecular structure.

The concepts of relaxation, chemical shift and coupling are related to one, two and three dimensional NMR experiments as a method for studying both molecular structure and properties. Practical applications of novel NMR experiments will also be discussed.