CHEM 629: Main Group Chemistry

(with special emphasis on solid-state NMR for materials characterization)

Fall 2020 SYLLABUS
MWF 1:35-2:25 pm, CHEM 2122

INSTRUCTOR: **Professor Dr. Janet Bluemel** — Reed McDonald building (RMD), rm 323 (via 321)
PHONE: 979-845-7749 | E-MAIL: bluemel@tamu.edu
Homepage: http://www.chem.tamu.edu/rgroup/bluemel/

OFFICE HOURS: **MWF 2:30 pm - 3:30 pm, or by appointment**

TEACHING ASSISTANT: **Fabian Arp —** RMD, room 428
PHONE: 979-862-7826 | E-MAIL: eberle@tamu.edu

TEXTBOOKS/COURSE MATERIAL:

Students will be provided with course material in the form of hardcopies or electronic files. This includes lecture scripts and exercise material, and the presented powerpoint files. It is no requirement, but helpful to have a textbook about the basics of NMR spectroscopy, such as the book by H. Friebolin, "Basic One- and Two-dimensional NMR Spectroscopy", or "Multinuclear NMR" by J. Mason, and a general Inorganic Chemistry textbook like C. E. Housecroft and A. G. Sharpe, or D. F. Shriver, P. W. Atkins, and C. H. Langford.

COURSE GRADING:

Will be determined once the students' backgrounds in the class are known. Participation in all lectures, discussions, and instrument demonstrations is expected. Additionally, the students will be provided with scripts for reading and powerpoint files for working on real life examples. There will be weekly homework sets that will be discussed in class. Students who are already active in research are encouraged to give short presentations about their work. Presenting recent literature and discussing its relevance with respect to the course will also count towards the grade.

The Final Exam will consist of a take home exercise which will be handed in within 10 days.

COURSE DESCRIPTION and LEARNING GOALS:

My aim is to provide a comprehensive and contemporary presentation of the diverse and fascinating discipline of inorganic chemistry. In this course we will focus on main group chemistry, with a special emphasis on solid-state NMR spectroscopy because the Department of Chemistry will get a new instrument soon. Solid-state NMR spectroscopy is indispensable for characterizing materials such as MOFs, zeolites, and molecular species adsorbed on or bound to solid surfaces. This also includes immobilized catalysts.

Main group elements range from highly reactive metals like lithium to noble gases, such as xenon, and most of them play important roles in NMR spectroscopy. The main group elements include solids, liquids and gases. Their chemistry and reaction mechanisms are highly interesting and to elucidate these, special emphasis will be placed on NMR and other spectroscopic techniques in this course. Modern analytical methods allow the thorough investigation of the diverse characteristics of inorganic molecules and materials. The purity of materials, dynamic effects, crystallographic features, and surface adsorption phenomena, for example, all play important roles in modern main group chemistry and this course will enable the students to fully understand the underlying principles.

Achievements in contemporary research, as well as industrial aspects of inorganic chemistry and spectroscopy are included. Examples taken from recent publications and seminar talks presented by visitors during the semester will be discussed.

In summary, the course Main Group Chemistry CHEM 629 this semester will have an emphasis on NMR spectroscopy. It will also cover modern one- and two-dimensional NMR techniques for liquids, such as DOSY, suspensions, and solids. In the foreground will be multinuclear and solid-state NMR applications on a wide range of compounds and materials that are interesting for inorganic chemistry, minerals, and polymers.

COURSE OUTLINE

I. For the Main Group Chemistry aspect of the course we will follow the Periodic Table

General topics include:

1. Structures of Solids

- Metals and Alloys
- Ionic Solids and Liquids
- Covalent compounds

2. Coordination Chemistry of Main Group Elements

- Ligands
- Constitution and Geometry
- Reactions and Applications of Coordination Compounds

3. Characterization Methods for Inorganic Compounds and Materials

- X-ray Powder and Crystal Diffraction
- EPR of Liquids and Solids
- IR, Raman, UV-VIS, Mass Spectrometry
- Photoelectron and Atomic Absorption Spectroscopy
- Mößbauer Spectroscopy

4. Selected Examples of Materials Chemistry in Academia and Industry

- Oxide Glasses and Pigments
- Layered Materials and Intercalation
- Metal Organic Frameworks (MOFs)
- Fullerides, Graphene, and Nanorods
- Inorganic Polymers
- Solid Catalysts and Surface Chemistry

II. NMR Spectroscopy of Liquids

1. The Basics of one- and two-dimensional NMR Spectroscopy

- the NMR experiment and the main functions of the NMR spectrometer
- the chemical shift and referencing with internal and external standards
- the *J*-coupling and standard correlation spectroscopy
- processing NMR spectra and preparing data for publications
- special pulse sequences and tricks

2. Multinuclear and oganometallic NMR spectroscopy

- the most common spin-1/2 nuclei, e.g. ^{19}F, ^{31}P, ^{29}Si, ^{119}Sn
- quadrupolar nuclei, e.g. ^{2}H, ^{6}Li, ^{11}B, ^{14}N

3. NMR of diamagnetic organometallic compounds

- peculiarities of ^{1}H/^{13}C chemical shifts
- different *J*-coupling scenarios and virtual couplings
- dynamic effects and ligand exchange

III. NMR Spectroscopy of Solids

1. Interactions in the solid state

- Chemical shift anisotropy
- Dipolar interactions
- Quadrupolar interactions

2. Description of the solid-state NMR spectrometer

- probeheads for Magic Angle Spinning (MAS)
- high-power decoupling and cross polarization (CP)
- equipment for special modern techniques, e.g. surface coils

3. Paramagnetic NMR spectroscopy

- the basics of paramagnetic compounds and their NMR
- metallocene catalysts
- applications for organometallic compounds and materials

IV. Most Recent Applications of Solution and Solid-State NMR

1. Homogeneous and heterogeneous catalysis

- HRMAS of suspensions (polymers, dendrimers, biomaterials, substances bound on surfaces)
- Dipolar Dephasing
- Diffusion Ordered Spectroscopy (DOSY)

2. Main Group Chemistry

- solid-state NMR of materials (metal organic frameworks (MOFs), chromatography phases)
- exchange processes and *in situ* reactions

The Americans with Disabilities Act (ADA) is a federal antidiscrimination statute that provides comprehensive civil rights protection for persons with disabilities. Among other things, this legislation requires that all students with disabilities be guaranteed a learning environment that provides for reasonable accommodation of their disabilities. If you believe you have a disability requiring an accommodation, please contact the Department of Student Life, Services for Students with Disabilities in Cain Hall, Rm. B118, or call 845-1637.

"*An Aggie does not lie, cheat or steal, or tolerate those who do*."