

Syllabus, Potential Lecture Topics, References

Called *Advances in Organic Chemistry* in the Online Schedule of Classes
AKA *Supramolecules and Assemblies: An Introduction*
Chemistry 504, Fall 2016,
Wright-Rieman Laboratories (Chemistry Building)
Tuesday & Thursday 5:00-6:20 PM, Wright-Labs Room 260
There are no prerequisites for this course

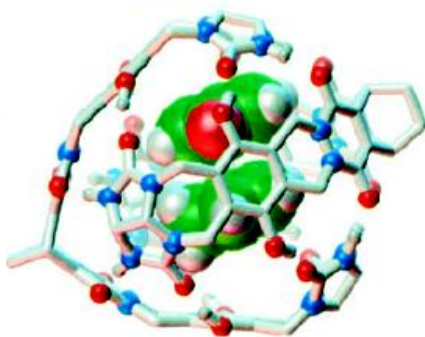
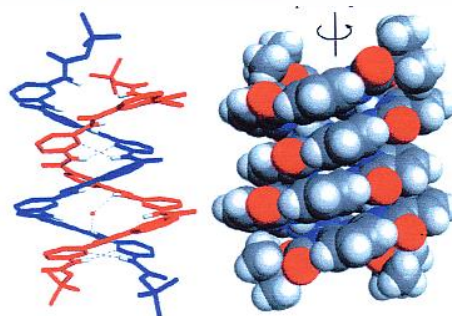
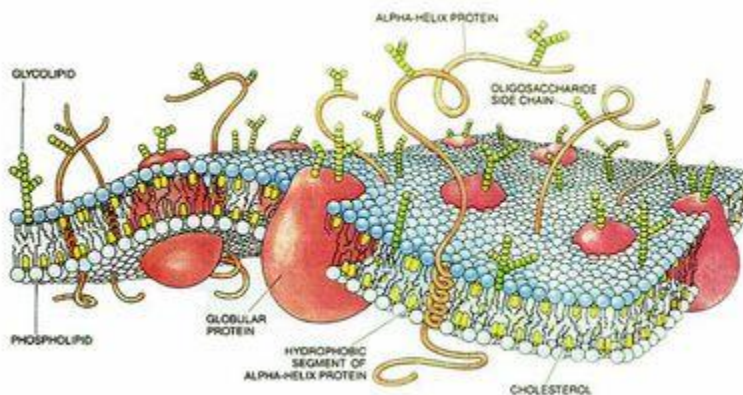
Instructor: Larry Romsted, Romsted@rutchem.rutgers.edu,
848-445-3639 (office), 732-247-0316 (home, emergencies), 732-325-4047 (cell)

Candy Corn Micelle in Space Video: https://www.youtube.com/watch?v=u_1RfqMH-KM
(additional interesting videos immediately follow this one)

Life depends on large structures, from enzymes with exquisite three-dimensional structures that catalyze reactions with extraordinary specificity and selectivity to biomembranes that are multi-component assemblies whose spontaneous formation is driven by the hydrophobic effect and held together by multiple weak interactions. Research in this field spans all disciplines and is expanding rapidly.

The goal of the course is to introduce the concepts and intellectual approaches to understanding the forces responsible for spontaneous assembly and to the logic to the creation of supramolecular aggregates for specific functions.

The semester will be divided into approximately two parts. One part will focus primarily on spontaneous surfactant self-assembly and topics will include the hydrophobic effect, association colloids, phase behavior, polyelectrolytes, chemical reactivity and applications from light harvesting to brushing teeth. The other part will introduce the interactions important for building supramolecular structures, host-guest chemistry, ion recognition, molecular encapsulation, interlocked systems, supramolecular chirality, catalysis and materials.



There are no prerequisites for this course and the level is suitable for advanced or entering graduate students and advanced undergraduates. The course will include lectures, assigned readings, problem assignments, longish quizzes/exams and a cumulative final. Each student will give an oral presentation on a topic from the current literature in the field toward the end of the semester. Course materials will be provided as handouts or online. No required books to purchase.

Probable Lecture Topics

Supramolecules

1. *Introduction*. Supramolecular Chemistry and Molecular Recognition. Concepts, Definitions, Language, Receptor Design Principles.
2. *Supramolecular Interactions*. Ion-ion interactions; Ion-dipole interactions; dipole-dipole interactions; hydrogen bonding; cation- π -interactions; π - π -interactions; van der Waals interactions; hydrophobic effect; metal-coordination bonds
3. *Host-Guest Chemistry*. Hosts for Cation Binding; Host for Anion Binding; Hosts for the Binding of Neutral Guests; Synthetic consideration; Templatation; Kinetic and Thermodynamic Aspects of Binding Selectivity
4. *Templates and Supramolecular Assemblies*. Programmed Supramolecular Systems; Kinetic and Thermodynamic Considerations; Self-assembled closed shell compounds; Helicates
5. *Supramolecular Chirality*. Chirality in Self-Assembled Systems; Chirality of Host-Guest Compounds; Chirality of Interlocked Systems.
6. *Supramolecular Reactivity and Catalysis*. Kinetic Models; Supramolecular Catalysts; Inner Phase Chemistry; Enzyme Models
7. *Self-Replicating Systems*. Kinetic Models; Self-replication in nature; Artificial Self-Replicating Systems
8. *Molecular and Supramolecular Devices*. Molecular Electronic Devices; Switches; Molecular Machines

Assemblies

1. *Introduction, Supramolecular Aggregates and Assemblies*. Types of surfactant spontaneous self-assemblies, micelles, microemulsions, vesicles; methods of characterizing of aggregate formation
2. *Forces contributing to spontaneous aggregation*. Surfactant formation and aggregate size and shape hydrophobic effect, interfacial interactions, salt effects
3. *Electrostatic Interactions*. Long range forces, also polyelectrolytes, surfactant aggregates and, binding of proteins to interfaces
4. *Phase Behavior in Surfactant Systems*. spherical, hexagonal, cubic, lamellar, etc. relation to surfactant structure determination of phase diagrams
5. *Chemical Reactivity in Association Colloids*. pseudophase model of chemical reactivity models distributions of organic molecules and ions
6. *Kinetic Treatments of Chemical Reactivity*. Spontaneous reactions, bimolecular and higher order reactions.
7. *Control of Reactivity in Surfactant Aggregates, and Cyclodextrins* (time permitting). Aggregates structure, micelles, vesicles (reaction and transport), DNA and drug delivery functionalized surfactants, mixed micelles, cyclodextrins

References (selected parts of some will be used as course materials, to be handed out)

Supramolecules

1. "Supramolecular Chemistry", Jean-Marie Lehn; 1st Ed. VCH, Weinheim, 1995.
2. "Supramolecular Chemistry", Jonathan W. Steed and Jerry L. Atwood, J. Wiley and Sons; 1st Ed. 2000.
3. "Principles and Methods in Supramolecular Chemistry", Hans-Joerg Schneider and Anatoly Yatsimirsky; J. Wiley and Sons; 1st Ed. 2000.

Assemblies

1. "Surfactants and Polymers in Aqueous Solution," B. Jönsson, B. Lindman, K. Holmberg, B. Kronberg, J. Wiley and Sons, 2nd Ed.
2. "Intermolecular and Surface Forces." J. Israelachvili, Academic Press, 2nd Ed. 1991
3. "The Colloidal Domain: Where Physics, Chemistry, Biology, and Technology Meet", D. Fennell Evans, H. Wennerström.
4. "Organic Reactivity in Microemulsions." C. A. Bunton, L. S. Romsted, *Handbook of Microemulsions Science and Technology*, Marcel Dekker, NY, 1999, p. 457-482
5. "Introduction to Surfactant Self-Assembly," Romsted, L. S. *Supramolecular Chemistry, from Molecules to Nanomaterials*, Gale, P.A., Steed, J.W., Eds., John Wiley & Sons, 2012., pp. 101-2003.
6. "Control of Reactivity in Aggregates of Amphiphilic Molecules." P. Scrimin, in *Supramolecular control of Structure and Reactivity*, John Wiley and Sons, 1996, Vol. 3, pp. 101-153.