Probing host-guest dynamic coupling using NMR spectroscopy and cryptophane inclusion complexes aligned in organic and aqueous liquid crystal solutions.

Physical Chemistry

Activities for participating students:

Host-guest inclusion complexes; cryptophanes; liquid crystals; ^{1}H, ^{2}H, ^{13}C, and ^{129}Xe NMR; cross-polarization; high-vacuum/gas handling; use of software packages including VNMR, MestreNOVA, MicroCal Origin, and Adobe Illustrator.

Project Description:

Of general interest is how (1) physical confinement at the nanoscale and (2) interactions between a guest and a host molecule affect the properties of a trapped molecule and the host/guest complex as a whole. Our studies use liquid-crystal (LC) matrices to amplify the interactions between nuclear spins of the involved molecules. For example, the signatures of interactions between host and guest molecules may be registered in LC-restored dipolar couplings, manifested either as splittings in the NMR spectra, or detected via magnetization transfer between guest and host spins; increases in structural/dynamical selectivity provide a new, direct probe of weak but specific interactions that underlie a host of chemical and biological phenomena. SEED participants will investigate the preparation, stability, ordering, and general NMR properties (e.g., chemical shifts, line splittings, and spin relaxation rates) of different LC solutions containing various complex-forming molecules to characterize the behavior of a given complex aligned within a LC environment. For example, cryptophanes are organic cage molecules that can be synthesized with varying cavity and portal sizes to allow fundamental studies of host-guest dynamic coupling (i.e., the relative motion of a guest within the host) via LCNMR. Finally, students will be trained on how to use our Varian Inova 400 MHz spectrometer, as well as various modern software packages involved in NMR data acquisition, processing, analysis, and presentation.

Mentor: Dr. Boyd Goodson