

Dept. of Chemistry and Biochemistry

Organic/Inorganic Seminar Series presents:



Orion B. Berryman

University of Montana

Friday, October 6, 2017

2:30–3:30 pm, 331 KLA

Coffee reception @ 2:00 pm, 377 KLA



Hosted by Darren Johnson

Halogen Bonding Strategies for Catalysis and Supramolecular Assembly

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The self-assembly of higher order anion helicates in solution remains an elusive goal. Here we present the first triple helicate to bind and encapsulate halides in organic and aqueous media, as well as the solid state. Fundamental studies of halogen bonding organic-catalysts lead us to develop a new paradigm to self-assemble higher-order helicates. Anion helicates self-assembles from three triply cationic arylolethynyl strands and resemble tubular anion channels lined with halogen bond donors. The triplexes exhibit remarkable stability at elevated temperatures being held together by nine inwardly directed halogen bonds and numerous buried π surfaces. We attribute this innovation to the stringent linearity of halogen bonding, in that the divergence of halogen bond donors along a helical axis destabilizes 1:1 complexation. In contrast, hydrogen bonding ligands capacity for binding halides is less dependent on bond angle. We hypothesize that incorporating halogen bonds within a simple alternating repeat unit can induce higher-order helication. Our initial studies on halogen bonding organocatalysts and current progress developing anion helicates into synthetic anion channels will be described.

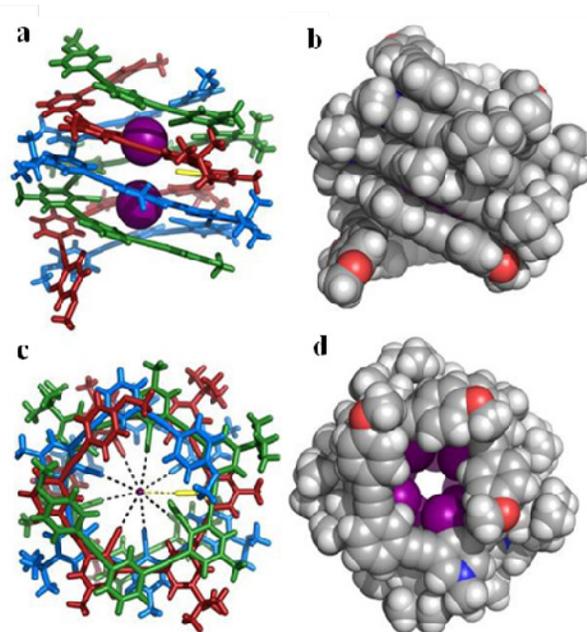


FIGURE 1: Solid-state structures of triple helicate. a, Tricolored stick representation of triple helicate. External iodide atoms removed for clarity. b, Side view space-filling representation of triple helicate, highlighting cylindrical and solvent-excluding shape. d, Top view of the encapsulation of two iodide atoms. e, Space-filling representation of triple helix, looking down anion channel (iodides removed).