



College of Liberal Arts and Sciences
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Synthetic Strategies toward Fluorosulfurylation of Organic Molecules and Sulfur-Fluoride Exchange (SuFEx)

Abstract: Sulfur-fluoride exchange (SuFEx) chemistry is emerging as a promising synthetic tool in chemical biology, material science, and synthetic chemistry. In synthesis, sulfur (VI) fluorides show unique promise as synthons in organic chemistry due their stability versus other sulfur (VI) halogen analogues. Key to the adoption of SuFEx chemistry is the development of efficient modes to synthesize and react sulfur (VI) fluorides. Research initiatives employing group 2, and transition-metal chemistry toward the synthesis of sulfonyl fluorides will be described. New SuFEx methods that react a broad set of S(VI) fluorides with carbon, oxygen, and nitrogen-based nucleophiles towards structurally diverse S(VI) compounds will also be presented.

A focus will be on a new SuFEx reaction to synthesize nitrogen-based sulfonylated compounds from a variety of S(VI) fluorides mediated via a Lewis acidic calcium salt will be described. Under a unified set of reaction conditions, sulfonyl fluorides, fluorosulfates, and sulfamoyl fluorides can be coupled with a variety of amines to synthesis a wide array of aryl and alkyl sulfonamides, sulfamides, and sulfamates in good to excellent yield. Computational and NMR kinetic studies that aim to elucidate the mechanism of Ca-activation will be discussed. Lessons learned from the mechanistic studies have led to preliminary data suggesting Ca-catalysis is possible.

Bio: Prof. Nicholas Ball grew up in Chattanooga, TN. He received his B.A. in Chemistry at Macalester College in 2005 and completed their Ph.D. in 2011 under Prof. Melanie Sanford at the University of Michigan working with C–F and C–CF₃ bond formation from high-oxidation state palladium. In 2010, he headed to the California Institute of Technology to pursue his postdoctoral studies with Prof. David Tirrell as a NIH Postdoctoral Fellow. Prof. Ball started as an Assistant Professor at Amherst College in 2013. In 2015 Prof. Ball joined the faculty at Pomona College and is now an Associate Professor of Chemistry with tenure. His current research focuses on developing new methods to make and use sulfur-based molecules that can be used for drug targets, chemical probes in biology, and material science. The work of his lab involves making molecules, machine learning, and computational chemistry. His work features

industrial, international collaborations as well as work with professors at other predominantly undergraduate institutions. Prof. Ball's honors and awards include Henry Dreyfus Teacher-Scholar Award and 2022 Chemical and Engineering News LGBTQ+ trailblazer. His research has been funded by NIH, NSF, and the American Chemical Society.