

DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE
SEMINAR SERIES
SPRING 2018

DATE: MONDAY, FEBRUARY 12, 2018

WHERE: CENTRAL KING BUILDING - 116

TIME: 11:30AM

GUEST SPEAKER

Dr. Pier Alexandre Champagne
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University of Ottawa

TOPIC

Developing and understanding organic reactions through experiments and computations

ABSTRACT

Understanding organic reaction mechanisms is a powerful way to identify new, and improve existing, chemical transformations. A combination of experimental and computational tools often yield better and more comprehensive insights than either individually. As such, two examples of mechanistic elucidations of organic reactions will be presented, where collaborative work between physical organic chemistry and density functional theory calculations was required to uncover the full picture. In the first part, the C-F activation of alkyl fluorides under neutral conditions will be discussed. We discovered that C-F bonds, which are inert under most reaction conditions, can be selectively activated through the use of appropriate hydrogen-bond donors. Different products and reaction mechanisms are observed when varying the activators and nucleophiles, leading to some unprecedented and sometimes unexpected reactivity. In the second part, a novel stereospecific rearrangement of homoallylic bromides will be highlighted. Our collaborators from the Feringa group discovered a dyotropic rearrangement involving a [1,2]-alkene shift leads to a regio- and stereospecific ring-contraction of bromocycloheptenes. This reaction proceeds under mild conditions, with or without a Lewis acid catalyst. Calculations show that the reaction occurs through a chiral non-classical cation-anion pair, which is crucial for the low activation barrier and selectivity.

Committee members:

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