

Department of Chemistry Seminar Series Spring 2023

Friday, April 14, 2023, 3:30 PM - HPA1-O119 (Health Sciences)

Ligand C=N Units in Molecular Materials Chemistry



Prof. David E. Herbert
Department of Chemistry and Manitoba Institute for Materials
University of Manitoba, Winnipeg Manitoba
Host: Prof. Titel Jurca

The C=N bond is a critical structural piece of many *N*-donor ligand scaffolds and is central to the properties and reactivity of a number of important coordination complexes - for example, promoting charge-transfer character in complexes of bipyridines (e.g., $[Ru(bpy)_3]^{2+}$) or the "redox non-innocence" of α -diimine complexes. Benzannulation can extend the conjugated C=N containing π -system of pyridine to quinoline (2,3-benzopyridine) to acridine (2,3-benzoquinoline), stabilizing the lowest unoccupied molecular orbital (LUMO) of the molecule and boosting electron-accepting properties, but the positioning of the benzannulation matters. For example, phenanthridine (3,4-benzoquinoline), an asymmetric isomer of acridine, bears a similarly electronically accessible extended π -system but more chemically isolated imine-like C=N moiety. In this presentation, the impact of such site-selective π -extension on the chemistry and properties of phenanthridine as a molecule and ligand will be discussed.

