

Nitrene Transfer Chemistry Mediated by First-row Transition Metal Complexes Supported by Macrocyclic Ligands

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**Chemistry
Seminar on Nitrene-
transfer reactions**

**Monday
Sept 28 at 4
pm in 126
Schrenk**

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Abstract: Nitrene-transfer reactions provide efficient routes to valuable nitrogen-containing compounds through C–N bond formation. Our work investigated how macrocyclic ligand design influences first-row transition-metal-catalyzed nitrene transfer using two catalyst platforms: pyridinophane-supported metal complexes and chiral tetraamido macrocyclic complexes.

In the first study, a series of M^{2+} ; $M = \text{Mn, Fe, Co, Ni, Cu}$ along with Cu (I) complexes supported by the pyridinophane ligand tBuN4 were evaluated as aziridination catalysts. Cu(I) and Cu(II) complexes exhibited the highest activity, while the remaining metal systems showed only modest reactivity. Mechanistic and computational studies support a stepwise aziridination pathway involving nitrene-centered radical intermediates, with the greater electrophilicity of the Cu(I)-derived nitrene accounting for its superior performance. DOI: <https://doi.org/10.3390/molecules30153097>

The second study describes the synthesis and characterization of a new family of chiral tetraamido macrocyclic Co(III) complexes. These catalysts promote aziridination and allylic amination reactions, particularly with less hindered styrenes. Mechanistic investigations indicate a stepwise pathway involving both polar and radical character, distinct from the behavior reported for related Co(TAML) systems. Mass spectrometric studies provide evidence for the formation of mono- and bis-nitrene cobalt intermediates under catalytic conditions. DOI: <https://doi.org/10.1021/acs.inorgchem.6c02795>

Overall, these studies demonstrate that macrocyclic ligand architecture strongly influences catalyst reactivity and mechanism, providing new insight into the design of selective and sustainable catalysts for aziridination and related nitrene-transfer reactions.

About the speaker: Himanshu Bhatia received his Bachelor of Science (honors) in Chemistry from University of Delhi, India in May 2015. He completed his Master of Science (H.S.) in Chemistry with specialization in Inorganic Chemistry from Panjab University in May 2017. He received his Ph.D from the Department of Chemistry at Missouri University of Science and Technology, Rolla, MO in July 2026 under the guidance of Dr. Pericles Stavropoulos. He specialized in synthetic organic & organometallic chemistry, and homogeneous catalysis. He received Outstanding Graduate Research Award (2026), Outstanding Graduate Service Award (2025), and Outstanding Graduate Teaching Assistant Award (2024) from the Department of Chemistry, Missouri S&T