

The Laboratory for Organic and Inorganic Chemistry

## Final PhD Seminar

Monday, June 23<sup>rd</sup> at 11:30

In Hall 1

**Mr. Liav Leiboviz**

Gandelman group

On the Topic of:

## **Positively Reactive: Naphthotriazinium Ligands in Transition Metal Complexes**

# Positively Reactive: Naphthotriazinium Ligands in Transition Metal Complexes

Name: Liav Leiboviz  
Supervisor: Prof. Mark Gandelman

The development of novel and non-innocent ligand frameworks is redefining what's possible in organometallic chemistry. In this seminar, I will present my Ph.D. research on a bold new class of cationic ligands—N-heterocyclic naphthotriazinium systems—that challenge conventional thinking in metal–ligand design. These ligands feature a highly electrophilic nitrenium core embedded within an extended  $\pi$ -aromatic naphthalene scaffold, unlocking a unique blend of tunable electronic properties and structural adaptability.

By integrating phosphine, pyridine, and amine donor arms, we created a modular platform that successfully coordinated to a wide range of transition metals. What makes these ligands truly exceptional is their ability to reversibly switch between classical L-type and unconventional Z-type bonding modes—rare behavior that we confirmed through crystallography, multinuclear NMR, and DFT analysis. This reversible duality isn't just unusual—it's unprecedented for a nitrogen-based ligand system.

But the chemistry doesn't stop there. These NHN ligands open the door to cooperative small-molecule activation. We achieved clean, selective activation of  $\text{H}_2\text{O}$ , and ammonia—two notoriously challenging substrates—via a unique bifunctional mechanism. The ligand and metal act in concert, flipping the expected polarity of bond activation (*umpolung* reactivity) and generating well-defined products with unexpected structure and behavior. These findings not only showcase the untapped potential of electrophilic ligand scaffolds but also hint at new directions in catalysis, bond activation, and redox-switchable design.

