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4324913 - Tantalum-catalyzed hydroaminoalkylation: A DFT study unveiling the role of metallacycle size | Poster Board #845

12:00 PM - 2:00 PM GMT-4

martedì, agosto 19, 2025

Room: Hall C (Walter E. Washington Convention Center)

Parent Session

Coordination Chemistry: Ligand Design, Synthesis, and Reactivity (/live/35/session/560462)

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DIVISION/COMMITTEE: [INOR: Division of Inorganic Chemistry] VIEW MORE ›

Organizer

Anna Svetlanova-Larsen, Ithaca College

Poster - In-person | INOR: Division of Inorganic Chemistry

Overview

Hydroaminoalkylation (HAA) is a powerful catalytic method for the direct functionalization of alkenes and alkynes with amines, garnering significant interest over the past decades. Among the effective catalysts, tantalum complexes featuring N,O-donor ligands with 4-membered metallacycles have demonstrated remarkable efficiency. Although previous studies shed light on important key steps of the mechanism, an investigation on a potential active role of the ligand during the reaction, as well as on the size of the metallacycle is still missing. In this study, we propose a computational mechanism of the tantalum-catalyzed HAA reaction, comparing the energy profiles for three catalysts: 4-, 5-, and 6-membered metallacycles (Scheme 1). Additional computational characterization tools allowed us to explain the observed trends. These findings rationalize the experimental results and provide a comprehensive new perspective on these systems, offering valuable understanding for the future development of catalysts within this family.

Presenter

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