Tantalum Metallacycle Size: A Key Determinant in Catalytic Efficiency for Hydroaminoalkylation Reactions

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Hydroaminoalkylation (HAA), a powerful catalytic approach for the direct functionalization of alkenes and alkynes with amines, has gained significant attention over the past decade.[1] Early transition metals such as Ti, Zr and Ta have been extensively utilized for HAA catalysis,[2] yet the development of efficient ligand systems to enhance the reactivity of these complexes remains a critical challenge. Among these, N,O-donor ligands[3] capable of forming 4-membered metallacycles[4] have demonstrated exceptional promise in improving catalytic performance. However, **a systematic investigation into the role of metallacycle size in dictating catalytic efficiency is still lacking**.

In this study, we designed and synthesized a series of Ta complexes featuring N,O-donor ligands that form 4-, 5-, and 6-membered metallacycles (Figure 1). These complexes were evaluated both experimentally and computationally for their activity in HAA reactions. Our findings offer valuable mechanistic insights into the influence of metallacycle size on catalytic performance, advancing the understanding of ligand design for expanded catalytic reactivity.

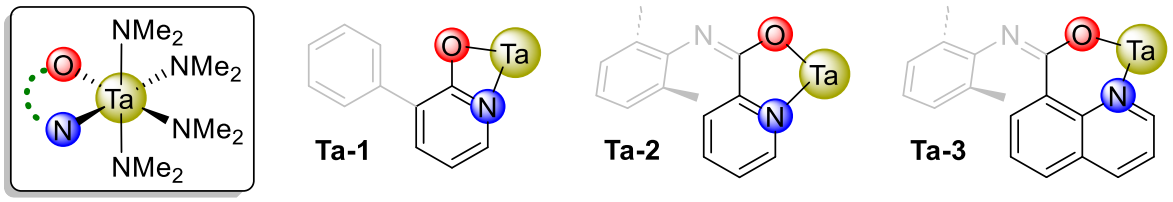


Figure 1. *Tantalum complexes featuring N,O-donor ligands forming 4-, 5-, and 6-membered metallacycles.*

References:

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