

Application of Indazolin-3-ylidenes in Catalysis: Steric Tuning of Nonclassical Formally Normal *N*-Heterocyclic Carbenes with Dual Electronic Character for Catalysis

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Rok wydania

2022

Czasopismo

Organometallics

Numer woluminu

41

Strony

1115-1124

DOI

10.1021/acs.organomet.2c00140

Kolekcja

Naukowa

Język

Angielski

Streszczenie

N-Heterocyclic carbenes (NHCs) are pivotal ligands in chemistry and catalysis, providing essential tools for the reactivity of metal centers. In particular, the development of nonclassical less heteroatom-stabilized *N*-heterocyclic carbenes (NHCs) has attracted tremendous attention owing to higher ligand basicity. However, research on the catalytic activity of nonclassical NHCs has been challenging due to restrictions in modifying steric environment crucial for catalysis. Herein, we report a new class of indazolin-3-ylidene ligands derived from readily available indazole that feature steric differentiation around the metal center. Compared to classical imidazol-2-ylidenes, these ligands feature strongly enhanced σ -donation resulting from re-positioning of one of the nitrogen atoms. Simultaneously, the presence of the fused aromatic ring results in strongly enhanced π -accepting properties. The % V_{bur} is higher than the classic imidazol-2-ylidene IMes ligand. We demonstrate that when used as ligands, the sterically differentiated coordination environment of indazolin-3-ylidenes efficiently promote the hydroamination reaction of alkynes to give valuable nitrogen-containing motifs, outcompeting the classical imidazol-2-ylidenes. This protocol has also been applied to the challenging hydrohydrazination of alkynes and applied to the late-stage diversification. Comprehensive characterization, coordination chemistry, as well as the evaluation of steric, σ -donating, and π -accepting properties are demonstrated. Computational studies to gain insight into the reaction mechanism are reported. We anticipate that sterically differentiated nonclassical indazolin-3-ylidenes will accelerate the development of well-defined less heteroatom-stabilized *N*-heterocyclic carbene ligands in transition-metal catalysis.

Typ publikacji

Artykuł

Słowa kluczowe

Catalysis, Differentiation, Hydrocarbons, Ligands, Organic reactions

Adres publiczny

<http://dx.doi.org/10.1021/acs.organomet.2c00140>

Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>

Plik został wygenerowany dnia 2026-10-14 17:05:53

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/aVvKAXB>.