

Wingtip-Flexible N-Heterocyclic Carbenes: Unsymmetrical Connection between IMes and IPr

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Streszczenie

IMes (IMes=1,3-bis(2,4,6-trimethylphenyl)imidazol-2-ylidene) and IPr (IPr=1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene) represent by far the most frequently used N-heterocyclic carbene ligands in homogeneous catalysis, however, despite numerous advantages, these ligands are limited by the lack of steric flexibility of catalytic pockets. We report a new class of unique unsymmetrical N-heterocyclic carbene ligands that are characterized by freely-rotatable N-aromatic wingtips in the imidazol-2-ylidene architecture. The combination of rotatable N-CH₂Ar bond with conformationally-fixed N-Ar linkage results in a highly modular ligand topology, entering the range of geometries inaccessible to IMes and IPr. These ligands are highly reactive in Cu(I)-catalyzed β -hydroboration, an archetypal borylcupration process that has had a transformative impact on the synthesis of boron-containing compounds. The most reactive Cu(I)-NHC in this class has been commercialized in collaboration with MilliporeSigma to enable broad access of the synthetic chemistry community. The ligands gradually cover %V_{bur} geometries ranging from 37.3 % to 52.7 %, with the latter representing the largest %V_{bur} described for an IPr analogue, while retaining full flexibility of N-wingtip. Considering the modular access to novel geometrical space in N-heterocyclic carbene catalysis, we anticipate that this concept will enable new opportunities in organic synthesis, drug discovery and stabilization of reactive metal centers.

Słowa kluczowe

Catalysis, Ligand Design, Metal Stabilization, N-Heterocyclic Carbenes, NHCs

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