

Bridged Pyrroloindole-CAYC-Gold Complexes: Harnessing Weak Secondary Intramolecular Au...H-C(sp³) Interactions in Gold(I) Catalysis

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Streszczenie

Gold(I) catalysis has been established as a tremendously powerful tool in organic synthesis and catalysis. Herein, we introduce a new class of electronically- and sterically-hindered N-heterocyclic carbene ligands, termed as bridged cyclic amino(ylide)carbene (^bCAYC), containing 9H-pyrrolo[1,2-a]indoles as the carbene core and diaryl sulfonium as the ylide partner. Highly electron-rich ^bCAYC ligands are suitable for synthesizing the corresponding gold(I) complexes, which exhibit a weak intramolecular Au...H-C(sp³) interaction as a secondary interaction where the gold d-orbitals act as electron donors and the C-H σ* orbitals act as acceptors. Properties and parameters of Au...H-C(sp³) interactions were investigated through X-ray, NMR, DFT, AIM, and NBO studies. This study reports a remarkably short Au...H-C(sp³) distance of 2.26 Å, as determined through X-ray crystallographic analysis. DFT and TEP data analysis revealed that ^bCAYCs are among the most σ-donating carbene ligands to date, than other widely used NHC ligands. The steric impact of ^bCAYCs has shown excellent potential for steric shielding, with %V_{bur} reaching up to 42.6%. These unique properties were well-reflected through the room-temperature hydroamination and one-pot C-N and C-C bond-forming reactions.

Słowa kluczowe

σ-donation, Au(I)-catalysis, Au...H-C(sp³) interaction, bridged cyclic (amino)ylide carbene, ligand design

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