

# Correlation of Ligand Donicity with Catalytic Activity in a Series of Gold (I) Carbene and Phosphine Complexes

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## Abstract

Catalytic activities of transition metal complexes are influenced by both steric and electronic effects arising from ancillary ligands. In the case of linear gold (I) complexes, the available evidence suggests that ligand electronic effects are more important. However, available methods to investigate the donor abilities of ligands are not easily conducted with gold (I) complexes. In this study, the donor abilities of selected carbene ligands, including N-heterocyclic carbenes (NHCs), abnormal N-heterocyclic carbenes (aNHCs), and acyclic diaminocarbenes (ADCs), as well as phosphine ligands, at a gold (I) center were studied. Methyl isocyanide adducts and 1,3-diisopropylbenzimidazolin-2-ylidene (*i*-Pr<sub>2</sub>-bimy) adducts of a series of gold complexes were synthesized as IR probes and <sup>13</sup>C NMR probes, respectively. The gold-catalyzed intramolecular cyclization of alkynes, which is known to be accelerated by strong donor ligands, showed an inverse relationship between the  $\nu_{\text{MeNC}}$  of the MeNC IR probe and the reaction rate. The same trend was observed with the <sup>13</sup>C NMR probe, but the MeNC IR probes gave a better correlation with catalytic rates. Explanations of the observed donicity trends in terms of bonding effects will be discussed.

**Keywords:** *Catalytic Activity, Gold (I) Carbene and Phosphine Complexes*