

CATALYSIS BY GOLD(I) COMPLEXES: LIGAND AND ANION EFFECTS

Paola Belanzoni*

Department of Chemistry, Biology and Biotechnology, University of Perugia,
Institute of Molecular Science and Technologies ISTM-CNR,
Consortium for Computational Molecular and Material Sciences (CMS)²
Via Elce di Sotto 8, 06123 Perugia, Italy
e-mail: paola.belanzoni@unipg.it

Gold(I) complexes have emerged in the last few years as excellent carbophilic Lewis acids that are able to activate the unsaturated C-C bonds (alkynes, allenes and alkenes) with outstanding efficiency towards the attack of a large variety of nucleophiles, thus enabling a broad range of transformations.^[1] The distinctive features of gold catalysis rely on the fact that reactions are promoted under milder conditions than other transition metal catalysts, lower temperatures, shorter reaction times and more tolerant to air and moisture and on attractive properties such as low toxicity and environmental benign nature. Several factors can potentially control the outcome of a gold-catalyzed reaction, such as the nature of the ligand, the use of additives, the choice of the counterion, the structure of the catalyst, etc. Abundant empirical information on these effects is now available, but a deep understanding is still lacking. The computational approach represents an important breakthrough towards a rational design of catalysts and reaction conditions, with ultimately predictive power. Based on DFT investigations, we provide here a clear picture of how ligands^[2] and anions^[3] influence the mechanisms of some key gold-catalyzed reactions.

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