

Modern Theoretical and Experimental Alchemy to Develop Sustainable & Green Homogeneous Gold(I) Catalysis

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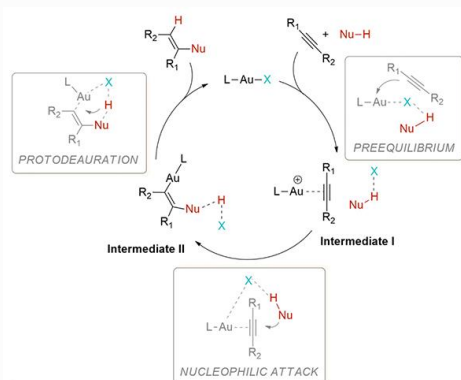
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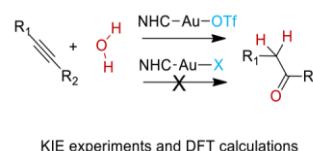
Abstract

Gold(I) cationic complexes of general formula $[LAu^+...X^-]$ [L = phosphines or NHCs (N-Heterocyclic Carbenes), X^- = anion] are successfully employed as catalysts in a large variety of organic reactions involving the activation of unsaturated carbon-carbon bonds. A key role in such reactions is played by the counterion, which strongly affects activity, regio- and stereo-selectivity. In literature, there are very few examples of gold homogeneous catalysis that works without silver additives, low catalyst loading, mild reaction conditions, simple work-up with the possibility of recovery the catalytic system, and using green solvents or even in neat condition.

In this contribution we report systematic experimental and theoretical data about the role of the anion in gold(I) catalysis by combining 1D and 2D multinuclear NMR spectroscopy and Density Functional Theory calculations. The overall experimental evidence, supported by computational results, confirms that the anion plays a crucial role in all steps of the reaction mechanism: pre-equilibrium, nucleophilic attack, and protodeauration. This complete rationalization of the counterion effect enabled us: 1) to develop a highly efficient methodology under solvent-, silver-, and acid-free conditions and 2) to replace traditional volatile organic compounds (VOC) with more eco-friendly green solvents.



- ➔ Solvent- | Silver- | Acid-FREE
- ➔ Room Temperature
- ➔ Reusability
- ➔ TON = 10^4 | TOF = 10^3 h⁻¹
- ➔ $E_{\text{factor}} = 0.03$ | EMY = 97



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