

## NEW RUTHENIUM AND COPPER COMPLEXES AS CATALYSTS OF C-C COUPLING REACTIONS OF ALKYNES

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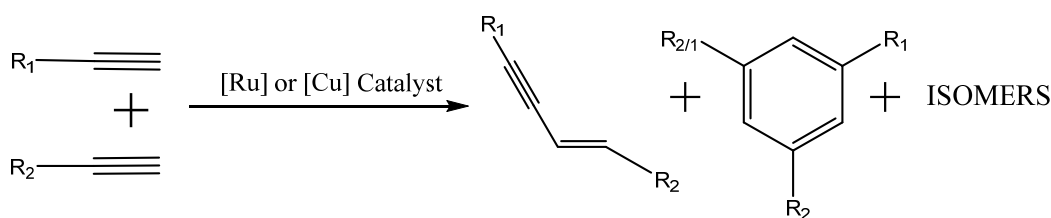
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Alkyne coupling is an important reaction in the synthesis of organic compounds due to its ability to form complex compounds, important precursors and products for the pharmaceuticals, agrochemical, and polymer industries. [1-3] Although C-C coupling reactions have become increasingly popular, they still present several challenges that must be overcome, for example, the tendency of alkynes to undergo homocoupling. Other challenges include the deactivation of the catalyst, the formation of undesired by-products due to the sensitivity of alkynes and the formation of mainly Z-alkenes. [4] For those reasons, and from a greener viewpoint (e.g., less energy consumption, easy catalyst availability and recovery, avoidance of toxic solvents/additives) the search for new catalysts and methodologies continues.

Phenylacetylene is often used as a model C-C coupling substrate due to its wide availability and its products are versatile building blocks in organic synthesis. [5] In this study, new ruthenium and copper complexes were tested as catalysts for phenylacetylene trimerization and dimerization reactions. Parameters such as temperature, solvent, type and amount of base, amount of catalyst and reaction time among others were optimized. In the end, C-C coupling reactions involving substituted substrates were also tested and compared in the optimized conditions.



- [1] J. Magano and J. R. Dunetz, "Large-scale applications of transition metal-catalyzed couplings for the synthesis of pharmaceuticals," *Chem. Rev.*, vol. 111, no. 3, pp. 2177–2250, 2011.
- [2] L. M. D. R. S. Martins, A. M. F. Phillips, and A. J. L. Pombeiro, "Chapter 8:C–C Bond Formation in the Sustainable Synthesis of Pharmaceuticals," *RSC Green Chem.*, vol. 2018-January, no. 54, pp. 193–229, 2018.
- [3] A. M. Trzeciak and A. W. Augustyniak, "The role of palladium nanoparticles in catalytic C–C cross-coupling reactions," *Coord. Chem. Rev.*, vol. 384, pp. 1–20, 2019.
- [4] M. Busch, M. D. Wodrich, and C. Corminboeuf, "A Generalized Picture of C-C Cross-Coupling," *ACS Catal.*, vol. 7, no. 9, pp. 5643–5653, 2017.
- [5] J. Zhong Jiang and C. Cai, "Pd/C catalyzed Sonogashira coupling reaction of phenylacetylene in TX10 microemulsion," *Colloids Surfaces A Physicochem. Eng. Asp.*, vol. 287, no. 1–3, pp. 212–216, 2006.