



TECHNOLOGY OFFER

Trifluoromethylcopper reagents from fluoroform.



ICIQ scientists have discovered a novel, highly sought after reaction: direct cupration of fluoroform (other names: trifluoromethane; HFC-23; R-23). Our exceedingly simple process employs only cheap reagents and is advantageously run at room temperature to produce CuCF_3 reagents that are useful in trifluoromethylation reactions. Partnership is offered for process optimization and adaptation to specific needs.

Give your projects a strong starting IP position:

At ICIQ, we consider that patents are safe and solid tools to provide protection from competitors. This is why we file patents for our developed technologies: to give our co-development projects with industry a **strong starting IP position**. As a research centre our goal is always to co-develop our technology **adapting it to the industrial partner's specific needs** and ultimately transfer the technology to this company, with a **flexible licensing strategy** adapted to each case.

We believe these elements are essential to a **healthy open innovation framework** and to a growing knowledge-based economy.

Chemical compounds bearing a trifluoromethyl group (CF_3) are widely used in the production of various pharmaceuticals and agrochemicals as well as specialty materials, polymers, composites, building blocks, and intermediates for various needs. However, the current manufacturing of trifluoromethylated compounds still needs improvements. Trifluoromethyl copper (I) compounds that are particularly useful in various trifluoromethylation reactions of organic molecules are conventionally made using costly CF_3 sources. Fluoroform, CF_3H , is an ideal source of CF_3 because it is inexpensive, readily available in large industrial quantities, non-toxic, and not an ozone depleter. However, the few known methods to prepare trifluoromethyl copper (I) compounds from fluoroform are all not only multistep and low-yielding, but also require low temperatures (-10 - -50 °C) to minimize the extremely facile decomposition of the highly unstable trifluoromethyl anion that is generated in the first, CF_3H deprotonation step. The ICIQ technology does not involve deprotonation of CF_3H . Instead, the CuCF_3 reagents are formed via direct cupration that is not mediated by the unstable trifluoromethyl anion and/or difluorocarbene. As a result, our CuCF_3 synthesis proceeds cleanly at room temperature while avoiding the formation of side-products. The trifluoromethyl copper reagents are obtained in high yield of up to >90% and can be used directly in various reactions, including aromatic trifluoromethylation. Treatment of a copper(I) source with 2 equivalents of an alkali metal alkoxide results in the formation of highly reactive dialkoxycuprates that directly metalate fluoroform to give CuCF_3 compounds in one step. These CuCF_3 reagents can then be used in various reactions with electrophiles to give trifluoromethylated products, including trifluoromethylated aromatic and heterocyclic derivatives.

Innovations and advantages of the offer

- clean production of trifluoromethyl reagents
- process works at room temperature and atmospheric pressure
- inexpensive and abundant trifluoromethyl source
- low-cost reagents

References

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