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Pd-Catalyzed Suzuki-Miyaura cross-coupling of aryl chlorides at low catalyst loadings in water

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PURPOSE OF THE ABSTRACT

The Suzuki-Miyaura cross-coupling reaction is the most employed transformation in industry for the formation of biaryl motifs. Although aryl iodides and/or bromides (electrophiles) allow this kind of transformation at very low catalyst loadings, the parental aryl chlorides do not participate in most of the reported cases. Recently, the use of water as solvent has drawn great attention due to its benign nature. However, additional organic solvents are still required, representing a potential drawback in industrial applications.

In the present work, the Suzuki-Miyaura cross-coupling reaction of electron-poor aryl chlorides in water is disclosed (Scheme 1).[1] Optimization of the reaction conditions allowed to run the reaction in water with 50 ppm of Pd-catalyst loading without any additional organic solvent. Kinetic studies revealed a very fast reaction rate, achieving high turnover numbers as well as turnover frequencies for the formation of biaryl products. Indeed, the organic substrate itself serves as a liquid organic phase in water, and the prone activation of the reagents over the two different phases accounted for the observed excellent reactivity. This biphasic behavior of the reaction has also been suggested and confirmed by dedicated control experiments. The reaction presented furthermore impressively robust scalability (up to 50 gram), giving the biaryl product in good yield and with a very low Pd-content.

FIGURES

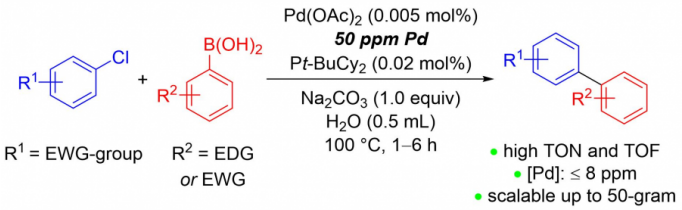

FIGURE 1

Suzuki-Miyaura cross-coupling of aryl chlorides

In water at 50 ppm catalyst loading

FIGURE 2

KEYWORDS

Suzuki-Miyaura | Cross-coupling | Pd-Catalyzed | Water

BIBLIOGRAPHY

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