

# Effects of Water on Iron-Catalyzed Cross-Coupling Reactions

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We have previously found that N-heterocyclic carbenes are effective ligands for the iron-catalyzed cross-coupling of primary and secondary alkyl Grignard reagents with non-activated aryl chlorides. However, after some time we began to notice some inconsistencies in the yields we obtained upon scaling up our reactions. One possible explanation was that trace water could have a beneficial effect on the reaction and the amount of trace water does not change proportionally as the reactions were run on a larger scale. To investigate this possibility, we performed the cross-coupling of isobutylmagnesium chloride with 4-chloroanisole using both anhydrous  $\text{FeCl}_2$  and  $\text{FeCl}_2 \cdot (\text{H}_2\text{O})_4$  as catalyst in the presence of an N-heterocyclic carbene ligand. The results shown below indicate that trace water is indeed beneficial in iron-catalyzed cross-coupling reactions.

