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IBzH (IBenzhydryl): sterically-flexible *N*-aliphatic *N*-heterocyclic carbenes (NHCs) for iron-catalyzed C(sp^3)–C(sp^2) cross-coupling of unactivated haloalkanes

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Streszczenie

Iron-catalyzed cross-coupling has emerged as a pivotal concept for the synthesis of valuable products across various facets of chemical research, including pharmaceuticals, organic materials and biological probes. In this respect, the use of N-heterocyclic carbenes (NHCs) as ancillary ligands to iron has been particularly effective. However, the major limitation is that the successful iron-catalytic systems have been almost exclusively limited to N-aryl-N-heterocyclic carbenes, which significantly restricts future developments of this commanding catalysis platform. Herein, we report IBzH (IBenzhydryl), a class of N-heterocyclic carbenes that are based on benzhydryl substitution of the imidazole ring. We demonstrate that this N-alkyl yet sterically-flexible ligand class promote the challenging C(sp^3)–C(sp^2) iron-catalyzed cross-coupling of unactivated haloalkanes, superseding the performance of other NHC ligands. Alkyl–alkyl cross-coupling is also described. Large scale synthesis and the evaluation of steric and electronic properties is presented. Considering the major advantages of sterically-flexible N-heterocyclic carbenes, we anticipate that this class of N-alkyl NHC ligands will have broad application.

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